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LINE-BY-LINE CALCULATION OF SPECTRA
FROM DIATOMIC MOLECULES AND ATOMS
ASSUMING A VOIGT LINE PROFILE

*by Ellis E. Whiting, James O. Arnold,
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*Ames Research Center
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SUMMARY

A Fortran IV computer program for predicting the spectra resulting from electronic transitions of diatomic molecules and atoms in local thermodynamic equilibrium is described in detail. Included are instructions for preparing the input data, a program listing, and complete flow charts. The program produces a spectrum by accounting for the contribution of each rotational and atomic line considered. The integrated intensity of each line is distributed in the spectrum by an approximate Voigt profile. The program can produce spectra for optically thin gases or for cases where simultaneous emission and absorption occurs. In addition, the program can compute the spectrum resulting from the absorption of incident radiation by a column of cold gas or the high-temperature, self-absorbed emission spectrum from a nonisothermal gas. The computed spectrum can be output directly or combined with a slit function and sensitivity calibration to predict the output of a grating spectrograph or a fixed wavelength radiometer.

INTRODUCTION

There are many applications in the field of quantitative spectroscopy where the ability to compute an emission or absorption spectrum is required. For example, electronic transition moments (or f-numbers) are often determined by comparing measured and computed intensities (see refs. 1-5). In such an application, test conditions giving an optically thin gas are usually required to simplify the problem, although Drake, Tyte, and Nicholls (ref. 5) recently reported a technique for determining these quantities from strongly self-absorbed spectra. Detailed spectral computations are also used in predicting radiative heat transfer in hot-gas environments, in stellar atmosphere calculations, for determining planetary surface pressure from measured line broadening, and for establishing basic spectroscopic constants.

The task of computing a reasonably accurate spectrum for a mixture of atoms and diatomic molecules is complicated by the enormously large number (often tens of thousands) of rotational lines forming the spectrum. In addition, several kinds of electronic transitions may be involved, each with its own required set of line strength and wavelength equations. These considerations make it impractical to produce the band spectra from even a simple

diatomic transition, such as $\text{BeO}(^1\Sigma \rightarrow ^1\Sigma)$, without the aid of an electronic computer. In response to this need, several computer programs have been written to produce synthetic spectra (see, e.g., refs. 5 and 6). However, most programs have been written for specific applications and cannot be applied to more general requirements. The present work was undertaken to develop a computer program applicable, to some degree of approximation, to any "allowed" electronic transition of diatomic molecules and atoms. Specifically, the program has the capability to include the following features in any computation:

1. Parallel transitions ($\Delta\Lambda = \Lambda' - \Lambda'' = 0$), in which spin splitting and lambda doubling are ignored (ignoring spin splitting and/or lambda doubling means herein that the total multiplet strength is assumed to reside in a single "effective" line),
2. Perpendicular transitions ($\Delta\Lambda = \pm 1$), in which spin splitting and lambda doubling are ignored,
3. $^2\Sigma \leftrightarrow ^2\Pi$ transitions, in which lambda doubling is ignored,
4. Atomic lines,
5. Option to terminate rotational-line calculations when the molecule dissociates due to rotation,
6. Option to include the alternation of line intensities for homonuclear molecules,
7. Use of an approximate Voigt profile for the line shape, and
8. Radiative energy transport in a nonisothermal gas.

The restrictions on spin splitting and lambda doubling can be removed with a modest reprogramming effort, but this would result in longer computer run times.

The output options available in the program are:

1. Tabulation of the spontaneous-emission spectrum (i.e., optically thin spectrum) for a 1.0 cm path length,
2. Tabulation of the "true" spectrum, which incorporates spontaneous emission, induced emission, absorption, and externally incident radiation through the equation of radiative transfer,
3. Tabulation of the curve of growth for an arbitrary number of wavelength intervals,
4. Tabulation of the integrated intensity over an arbitrary number of wavelength intervals, and

5. Tabulation of the output signal produced by a radiometer or spectrometer by specifying an instrument calibration. The instrument slit function can be approximated by up to 99 straight-line segments or by a Gaussian curve. The computation can be made at a fixed wavelength to simulate a radiometer or by scanning across any specified wavelength interval to simulate a grating instrument. In the latter case, the sensitivity can be varied as a function of wavelength to accurately simulate a grating-instrument calibration.

The computer program presented is also discussed in reference 7. That reference describes the theoretical and numerical assumptions made in the program, compares computer results with those given by other programs, and demonstrates the flexibility of the program in solving a wide variety of problems. However, that paper does not discuss programming details and, consequently, is not in a useful form for understanding and using the program. This paper provides: (1) a discussion of program operations, (2) a listing of the program statements, (3) detailed flow charts of the program logic, and (4) a guide for preparing the input data necessary to operate the program. It is assumed that the reader has a copy of reference 7 available; therefore, the information contained in that paper will not be reproduced herein.

The program is available from COSMIC, Barrow Hall, University of Georgia, Athens, Georgia. The program package includes the program source decks, an 800 BPI magnetic tape with spectroscopic data for 18 diatomic systems, and the input and output for an extensive program checkout. When requesting this program, refer to Flash Sheet number ARC-10221.

SYMBOLS

<u>FORTTRAN IV</u>	<u>Commonly Used Notation</u>	
ALPHA	α_e	rotational constant for equilibrium position, cm^{-1}
ALTNAT		alteration factor for homonuclear molecules, dimensionless ALTNAT = 0, lines do not alternate in intensity = 1, lines with K'' odd are strongest = 2, lines with K'' even are strongest
ATOMCC		number density of atoms, atoms-cm^{-3}
BE	B_e	rotational constant for equilibrium position, cm^{-1}
BE X B-X	$\text{BeO}, B^1\Sigma \rightarrow X^1\Sigma$	band system for BeO molecule near 4700 Å
BETA	β_e	rotational constant for equilibrium position, cm^{-1}
BLAM	B_λ, B_λ^0	Planck or black-body function, $\text{W-cm}^{-2}\text{-}\mu^{-1}\text{-sr}^{-1}$

BV	B_v	rotational constant for the vibrational level v , cm^{-1}
CAPA	A	spin coupling constant, cm^{-1}
CAPL	Λ	quantum number specifying the component of the resultant electronic angular momentum along the internuclear axis, dimensionless
CH3900	$\text{CH}, B^2\Sigma \rightarrow X^2\Pi$	band system of CH molecule near 3900 Å
CH4300	$\text{CH}, A^2\Delta \rightarrow X^2\Pi$	band system of CH molecule near 4300 Å
CINT3		intensity factor defined in equation (12) page 12
CN V	$\text{CN}, B^2\Sigma \rightarrow X^2\Sigma$	violet band system of CN molecule
CN RED	$\text{CN}, A^2\Pi \rightarrow X^2\Sigma$	red band system of CN molecule
CØASDI	$\text{CO}, a'^3\Sigma \rightarrow a^3\Pi$	Asundi band system of CO molecule
CØ+ CT	$\text{CO}^+, A^2\Pi \rightarrow X^2\Sigma$	comet tail band system of CO molecule
CØ 4+	$\text{CO}, A^1\Pi \rightarrow X^1\Sigma$	fourth positive band system of CO molecule
CONST1 CONST2 CONST3	}	constants used in line strength expressions in sub-routine S2 PI2 and specified in table I
CSPRD1 CSPRD2 CSPRD3	}	constants used in Voigt profile expressions and defined in equations on page 11
CSTR		constant used in line strength expression in sub-routine ZERO and defined in equation on page 14
C2PHIL	$\text{C}_2, b^1\Pi \rightarrow a^1\Sigma$	Phillips band system of C_2 molecule
C2SWAN	$\text{C}_2, A^3\Pi \rightarrow X^3\Pi$	Swan band system of C_2 molecule
DE	D_e	rotational constant for equilibrium position, cm^{-1}
DEGEN	d	electronic multiplicity, dimensionless
DELLAM	$\Delta\lambda$	distance between wavelength locations at which spectrum is computed, Å
DEPTH	l, x	depth of radiating gas, cm
DV	D_v	rotational constant for the vibrational level v , cm^{-1}
DZERO	D_0	dissociation energy referred to the $v = 0$ vibrational level, cm^{-1}

E	E, I	line integrated spontaneous emission, $\text{W-cm}^{-3}\text{-sr}^{-1}$
E	$G(v)+F(K)$	sum of vibrational and rotational energy used in iteration to find KMAX and defined by equation (15) on page 13
EINSTN	A_{ul}	Einstein A coefficient, probability of transition, $\text{sec}^{-1}\text{-part}^{-1}$
ELAM(M)	E_{λ}, I_{λ}	spectral intensity distribution of spontaneous emission, $\text{W-cm}^{-3}\text{-}\mu^{-1}\text{-sr}^{-1}$
FRANCK	q_v, v''	Franck-Condon factor, dimensionless
IFACTR		integer name of the intensity factor, CINT3, set up in Hollerith mode so that if CINT3 = 0.0 blanks are printed rather than zeros
ILAM(M)	I_{λ}, B_{λ}	specific intensity, $\text{W-cm}^{-2}\text{-}\mu^{-1}\text{-sr}^{-1}$
J	J	rotational quantum number, dimensionless
K	K, N	rotational quantum number without spin, dimensionless
KMIN	K_{\min}	minimum rotational quantum number, dimensionless
KMAX	K_{\max}	maximum rotational quantum number, dimensionless
LAM(M)	λ	wavelengths specifying incident spectrum array or linear segment slit function, Å
LAMBDA(M)	λ	wavelength locations at which spectrum is computed, Å
LAMCL	λ_{CL}	center of rotational or atomic line or location of center of slit function, Å
LAMMIN	λ_{\min}	minimum wavelength in computed spectrum, Å
LAMMAX	λ_{\max}	maximum wavelength in computed spectrum, Å
LAMR(M)	λ	wavelengths specifying instrument calibration, Å
LAMS(M)	λ	wavelengths at which instrument output signal is generated, Å
LAMS1	λ	starting wavelength for scanning slit or wavelength for fixed linear slit Å
LAMS2	λ	stopping wavelength for scanning slit, Å
LAM1	λ	starting wavelength for spectral integration, Å
LAM2	λ	stopping wavelength for spectral integration, Å

LEVELS		number of electronic energy levels for a diatomic molecule
MU	μ_A	reduced mass in atomic-weight units
NAME		six-letter (or less) name specifying an atomic or diatomic system
NARRAY		number of points at which spectrum is computed
NCENTR		array index in ELAM(M) nearest to center of line being added to spectrum
NEND		array index in ELAM(M) at which the last contribution of a line is added
NINTRV		number of intervals in a case over which the spectrum will be integrated
NPOINT		number of array elements specifying the slit function. NPOINT = 0 if the slit function is specified by a Gaussian curve
NRLAMS		number of points specifying the instrument calibration
NSLIT		number of slits for which the instrument output signal will be computed
NSPRED		one-half the number of places in the spectrum to which a line will be added
NSTART		array index in ELAM(M) at which the first contribution of a line is added
NUBAR	$\bar{\nu}$	wave number of a line center, cm^{-1}
NUBARO	$\bar{\nu}_0(v'v'')$	wave number of a band origin, cm^{-1}
NUSPIN	N,I	nuclear spin of an atom in a homonuclear diatomic molecule, dimensionless
N2LBH	$\text{N}_2, a'^1\Pi \rightarrow X^1\Sigma$	Lyman-Birge-Hopfield band system of N_2 molecule
N2 1+	$\text{N}_2, B^3\Pi \rightarrow A^3\Sigma$	first positive band system of N_2 molecule
N2 2+	$\text{N}_2, C^3\Pi \rightarrow B^3\Pi$	second positive band system of N_2 molecule
N2+ 1-	$\text{N}_2^+, B^2\Sigma \rightarrow X^2\Sigma$	first negative band system of N_2^+ molecular ion
NØ B	$\text{NO}, B^2\Pi \rightarrow X^2\Pi$	beta band system of NO molecule
NØ G	$\text{NO}, A^2\Sigma \rightarrow X^2\Pi$	gamma band system of NO molecule
Ø2 SR	$\text{O}_2, B^3\Sigma \rightarrow X^3\Sigma$	Schuman-Runge band system of O_2 molecule
ØH3060	$\text{OH}, A^2\Sigma \rightarrow X^2\Pi$	band system of OH molecule near 3060 Å

PARTCC	N	number density of molecules, molecules-cm ⁻³
Q	Q	partition function, dimensionless
R	r	internuclear distance, cm
RANGE		number of line widths from the line center that a line is added to the spontaneous emission spectrum, integer
RE	r _e	internuclear distance at equilibrium position, cm
RLAM(M)		spectral calibration of scanning slit that multiplies slit function to yield instrument sensitivity
RLAMCL		value of spectral calibration RLAM(M) at slit centerline, LAMCL
RMAX		maximum value of RSLIT(M)
RSLIT(M)		slit function values for linear segment slit function
SCAN		flag to indicate whether a fixed slit (SCAN ≠ 1) or a scanning slit (SCAN = 1) is specified
SIGN		constant used in line strength expressions in subroutine ONE and in equations (19), (20), and (21) on page 15, dimensionless
SIGNAL		instrument output signal computed in subroutine SLIT, arbitrary units
SIGNS1 } SIGNS2 } SIGNS3 }		constants used in line strength expression in subroutine S2 PI2 and in equations (23) and (24) on pages 15 and 16, dimensionless
SIGNU1 } SIGNU2 }		constants used in NUBAR expression in subroutine S2 PI2 and in equation (22) on page 15, dimensionless
STEP		wavelength interval between points where the instrument output signal is computed for a scanning slit, Å
SUMRE2	$\sum R_e(\vec{r}_{v',v})/ea_0 ^2$	sum of the squares of the dimensionless electronic transition moments. The sum is over all electronic transitions from the upper and lower multiplet levels
TELECT	T _{elect}	electronic temperature, °K

TERM(M)	T_e	electronic term energy, cm^{-1}
TOTALI		integrated spectral intensity, over a specified wavelength interval, found in subroutine INTRVL, $\text{W-cm}^{-2}\text{-sr}^{-1}$
TROT	T_{rot}	rotational temperature, $^{\circ}\text{K}$
TVIB	T_{vib}	vibrational temperature, $^{\circ}\text{K}$
U	U	molecular potential energy defined in equation (13) on page 13, cm^{-1}
V	v	vibrational quantum number, dimensionless
WIDTH		width of Gaussian slit function at half-peak or width of linear segment slit function defined by equation (27) on page 16, \AA
WIDTHG	w_g	width of Gaussian line profile at half-height, \AA
WIDTHL	w_l	width of Lorentzian line profile at half-height, \AA
WIDTHV	w_v	width of Voigt line profile at half-height, \AA
WE	ω_e	vibrational spectroscopic constants, cm^{-1}
WEXE	$\omega_e x_e$	
WEYE	$\omega_e y_e$	
WEZE	$\omega_e z_e$	
Y	Y	ratio of spin coupling constant to rotational constant for given vibrational level (A/B_v), dimensionless
U	$()', ()_u$	letter following many of the above symbols to indicate upper level (i.e., $\text{ALPHAU} \equiv \alpha'_e$)
L	$()'', ()_L$	letter following many of the above symbols to indicate lower level (i.e., $\text{ALPHAL} \equiv \alpha''_e$)
\emptyset	O	the capital letter O, when appearing in band-system names

PROGRAM DESCRIPTION

A listing of the program, liberally annotated with comment statements, is provided in appendix A. This listing, in direct association with the flow charts of each subroutine given in appendix B, provides a complete and detailed description of the program. A simplified flow chart of the main program, illustrating the step-by-step flow through the program, is shown in figure 1. This simplified flow chart should be studied carefully to keep the overall program logic clearly in view. In addition, the following discussion is included to aid the reader in understanding the program.

The end result of this program is to produce the "true" spectrum as given by the equation of radiative transfer. Within the computer the "true"

spectrum is generated in two distinct steps. In the first step the spectrum due to spontaneous emission only is computed. This is accomplished by summing the spectral contributions from all included lines at many points within the spectral range considered. For atomic lines this is accomplished entirely within the ATOMIC subroutine. For diatomic molecules the procedure is somewhat more complicated. When a new band system is specified, program control is transferred to the SETUP subroutine. In this subroutine, the spectroscopic constants are read either from cards or from magnetic tape and the partition function, Q , is computed. After these tasks are completed, control is transferred back to the main program where a vibrational band card is read. This card causes control to be transferred to the VU VL subroutine where: (1) the appropriate vibrational constants are computed from the spectroscopic constants, (2) an intensity factor (CINT3) is computed if needed, and (3) the maximum rotational quantum number is found. After these tasks are completed, control is transferred back to the main program, followed by an immediate transfer to the appropriate rotational-structure subroutine, ZERO, ONE, or S2 PT2. Subroutine ZERO applies to parallel transitions, subroutine ONE applies to perpendicular transitions, and subroutine S2 PT2 applies to $^2\Sigma \rightarrow ^2\Pi$ or $^2\Pi \rightarrow ^2\Sigma$ transitions. In these subroutines, the wavelength and integrated intensity due to spontaneous emission of each rotational line are calculated, the intensity is distributed spectrally into a Voigt profile, and the line is added into the spectrum.

If several vibrational bands are specified for several band systems, the summation process can include tens of thousands of rotational lines. The resultant spectral sum of this multitude of lines, including any atomic lines specified, yields the spontaneous-emission spectrum. If an optically thin spectrum is desired as a final result, it is given directly by the spontaneous-emission spectrum.

The second step in the development of the "true" spectrum is to compute the wavelength-dependent absorption coefficient, including induced emission. As described in reference 7, this function is given directly by dividing the spectral intensities due to spontaneous emission, developed above, by the Planck (or black body) function at the appropriate temperature and wavelengths. The absorption coefficient is then combined with the geometric gas depth and the incident radiation, if specified, in the equation of radiative transfer to give the "true" spectrum.

The generality of the program is greatly enhanced by permitting the "true" spectrum radiating from a gas layer to be used as the incident radiation for a new gas layer. This allows the calculation of the "true" spectrum from a multilayer source, where each layer is specified by a different thermochemical and thermodynamic environment.

Most of the numerical steps performed in the program can be easily understood once the intent of the operation is known. The comment statements in the listing and the description of the theory given in reference 7 should make the intent of most operations clearly evident. There are, however, a few operations that need additional discussion. These are presented in the following sections.

Spontaneous-Emission Spectrum

The procedure for building the spectrum involves several steps. These steps will be easier to understand if the notation illustrated in figure 2 is followed closely during the discussion. A large array (ELAM(M)) with 9000 entries is reserved in the computer core for summing the spectral intensity at many points within the spectral range considered. The minimum (LAMMIN) and maximum (LAMMAX) wavelengths are specified as is the wavelength interval (DELLAM) between points where the spectrum is to be summed. For good spectral resolution, DELLAM is normally selected to be about 1/10 of the narrowest line width at half-height (WIDTHV) considered in the calculation.

The total number of points at which the spectrum is summed (NARRAY) is limited to 9000. NARRAY is found from LAMMIN, LAMMAX, and DELLAM, and, if NARRAY is greater than 9000, DELLAM is changed so that NARRAY is equal to 9000. LAMMAX is always recomputed to ensure that it is exactly an even increment of DELLAM from LAMMIN. For this reason, the value of LAMMAX used and output by the program may be slightly less than the value input.

The contributions from each rotational and atomic line to the spontaneous emission spectrum are added into the ELAM(M) array by the following procedure. The array index number nearest to the line center (NCENTR) is found from (refer to fig. 2)

$$NCENTR = \left(\frac{LAMCL - LAMMIN}{DELLAM} + 1.5 \right)_{\text{truncated}} \quad (1)$$

where LAMCL is the wavelength of the line center, and the characteristic of Fortran IV to convert real numbers into integer numbers by rounding down (truncating) has been used.

Theoretically, each line makes a contribution to the spectrum at all wavelengths. Beyond some distance from the line center, however, the contribution of the line to the spectral intensity is very small. Therefore, computer run time can be reduced considerably, with slight loss in accuracy, by adding each line into the spectrum for only a limited distance from the line center. In the program, this distance is specified by RANGE, in terms of a given number of line widths.

If RANGE is input as zero (or the card field is left blank) then RANGE is set as follows: For a pure Gaussian line profile, the spontaneous-emission intensity is less than 10^{-11} of the peak line intensity only three line widths from the line center. Therefore, RANGE = 3.0 is considered adequate for this case. For a Lorentzian or Voigt line profile the intensity in the wings is much stronger than for a Gaussian profile, and RANGE is increased to 5.0 for these cases. This limitation results in approximately 5 percent of the spontaneous integrated intensity being excluded from the computation for a pure Lorentzian line profile.

The number of entries in the ELAM(M) array from the location defined by NCENTR, to which contributions from a given line are added, is

$$\text{NSPRED} = \left(\frac{\text{RANGE} \cdot \text{WIDTHV}}{\text{DELLAM}} + 1.1 \right)_{\text{truncated}} \quad (2)$$

The array indices that define the first (NSTART) and the last (NEND) entries in the ELAM(M) array to which a contribution from a line is added is

$$\text{NSTART} = \text{NCENTR} - \text{NSPRED} \quad (3)$$

$$\text{NEND} = \text{NCENTR} + \text{NSPRED} \quad (4)$$

These indices provide limits for a simple DO loop, involving the line-profile expression (see refs. 7 and 8), which adds the contributions from each line to the correct locations in the ELAM(M) array, and hence forms the spontaneous-emission spectrum. In partial Fortran IV notation, the line-profile expression from reference 8 can be written

$$\begin{aligned} \text{ELAM}(M) = E \left[\text{CSPRD1} \cdot e^{-2.772 \cdot \text{CSPRD3}^2} + \frac{\text{CSPRD2}}{1 + 4 \cdot \text{CSPRD3}^2} \right. \\ \left. + 0.016 \cdot \text{CSPRD2} \left(1 - \frac{\text{WIDTHHL}}{\text{WIDTHV}} \right) \left(e^{-0.4 \cdot \text{CSPRD3}^{2.25}} - \frac{10.0}{10 + \text{CSPRD3}^{2.25}} \right) \right] \quad (5) \end{aligned}$$

where E is the integrated spontaneous emission of the line and

$$\text{CSPRD1} = \frac{[1 - (\text{WIDTHHL}/\text{WIDTHV})] \cdot 10^4}{\text{WIDTHV}[1.065 + 0.447(\text{WIDTHHL}/\text{WIDTHV}) + 0.058(\text{WIDTHHL}/\text{WIDTHV})^2]} \quad (6)$$

$$\text{CSPRD2} = \frac{(\text{WIDTHHL}/\text{WIDTHV}) \cdot 10^4}{\text{WIDTHV}[1.065 + 0.447(\text{WIDTHHL}/\text{WIDTHV}) + 0.058(\text{WIDTHHL}/\text{WIDTHV})^2]} \quad (7)$$

$$\text{CSPRD3} = \left| \frac{\text{LAMBDA} - \text{LAMCL}}{\text{WIDTHV}} \right| \quad (8)$$

LAMBDA is the wavelength at which the spectrum is computed

$$= \text{LAMMIN} + (M - 1) \cdot \text{DELLAM} \quad (9)$$

Intensity Factor

The first major step taken in the program for any spectral computation is to generate the spontaneous-emission spectrum as outlined above. When spontaneous emission from a cold gas is computed, however, the intensities are

numerically small because of the low concentration of molecules in the upper state. The expression for the number of molecules in the upper state is given by (see ref. 7)

$$N_u = \frac{N_d(2J' + 1)e^{-\frac{hc}{k} \left(\frac{T_e'}{T_{elect}} + \frac{G'}{T_{vib}} + \frac{F'}{T_{rot}} \right)}}{Q} \quad (10)$$

The exponent will be a large negative number for high term energies and/or low temperatures. For example, in the case of the $A^1\Pi$ state of CO at room temperature, the electronic and vibrational part of the exponent is approximately -300. The computer cannot recognize numbers less than $10^{-38} = e^{-87.5}$ and simply equates all numbers less than this value to 0.0. Therefore, a straightforward application of the above equation to CO(4+) at room temperature would produce meaningless numbers.

To overcome this computer-caused limitation, an intensity factor is introduced as follows:

$$\bar{N}_u = N_u \cdot 10^{CINT3} = \frac{N_d(2J' + 1)e^{-\frac{hc}{k} \left(\frac{T_e'}{T_{elect}} + \frac{G'}{T_{vib}} + \frac{F'}{T_{rot}} \right) + 2.30259 \cdot CINT3}}{Q} \quad (11)$$

where

$$CINT3 = \left\lfloor \frac{\frac{hc}{k} \left(\frac{T_e'}{T_{elect}} + \frac{G'}{T_{vib}} \right)}{2.30259} \right\rfloor \text{ truncated} \quad (12)$$

From these expressions, it is clear that CINT3 is an even power of 10 that adjusts the numerical value of N_u into a numerically acceptable regime. Results that include the intensity factor are obviously in error by this factor and it must be removed before the results can be used. When numbers reflecting only spontaneous emission are printed, the correction is applied at the time of printing. For example, suppose an exact intensity of 3.5×10^{-178} should have been computed, but an intensity factor of 10^{+170} was applied. The value found by the program is, therefore, 3.5×10^{-8} , but is printed as $3.5 \times 10^{-8} \times 10^{-170}$. In printer notation this appears as 3.500E-08-170. The intensity factor is printed by using the Hollerith array, IFACTR, so that, when the intensity factor is zero, blanks will appear on the printed output rather than zeros. When the "true" spectrum is computed, the intensity factor is removed from the calculation at the time the absorption coefficient is computed and no further correction is necessary.

Maximum Rotational Quantum Number (KMAX)

A rotating molecule develops a centrifugal force that distorts the potential well. If the nonrotating potential well is described by a Morse potential, then the rotation-dependent potential is given by (see ref. 9)

$$U = D_e \left[1 - e^{-\beta(R-R_e)} \right]^2 + \frac{hK(K+1)}{8\pi^2 c \mu R^2} \quad (13)$$

where

$$\left. \begin{aligned} \beta &= (2\pi^2 c \mu / D_e h)^{1/2} \omega_e \\ \mu &= \text{reduced mass, g} \end{aligned} \right\} \quad (14)$$

The effect of rotation on the potential well can be seen by the curves in figure 3 for HgH taken from reference 9. The molecule will dissociate when the vibrational plus rotational energy equals or exceeds the rotation-induced local maximum in the potential well.¹ The sum of the vibrational and rotational energies is given by

$$\begin{aligned} E &= \omega_e(v + 1/2) - \omega_e x_e(v + 1/2)^2 + \omega_e y_e(v + 1/2)^3 + \omega_e z_e(v + 1/2)^4 \\ &+ B_v K(K+1) - D_v K^2(K+1)^2 \end{aligned} \quad (15)$$

Therefore, once a vibrational level has been specified, an iteration scheme is required to find KMAX from equations (13) and (15).

The energy of the local maximum can be found from equation (13) if the rotational quantum number and the internuclear distance (R) at that point are known. The internuclear distance at the local maximum is found for a specified value of K by differentiating equation (13) and equating it to zero, that is,

$$\frac{dU}{dR} = 2D_e \beta \left[1 - e^{-\beta(R-R_e)} \right] e^{-\beta(R-R_e)} - \frac{2hK(K+1)}{8\pi^2 c \mu R^3} = 0 \quad (16)$$

For numerical solution, this equation is rewritten as

$$f(R) = R^3 \left[1 - e^{-\beta(R-R_e)} \right] e^{-\beta(R-R_e)} = \frac{hK(K+1)}{8\pi^2 c \mu D_e \beta} = g(K) \quad (17)$$

and is illustrated in figure 4.

¹In fact, some predissociation will occur at lower energies due to a wave mechanical passage through the potential barrier, but this effect is ignored in the present program.

The value of R at the local maximum, R' , is found by stepping R from its equilibrium value (R_e) by fixed increments (0.1×10^{-8} cm) until $f(R)$ exceeds and then falls below $g(K)$; R' is then found by interpolating to $f(R) = g(K)$. If $f(R)$ passes its maximum before $g(K)$ is reached, the rotational quantum number is too large and rotational dissociation would have occurred. A local maximum in the potential well does not exist in this case (see curve for $K = 40$ in fig. 3), but a value of R at or near the peak of the $f(R)$ curve is chosen for the iteration.

Once the internuclear distance for the local maximum is found (at the specified rotational quantum number) it is combined with the vibrational quantum number to compute the values of U and E from equations (13) and (15). When the iteration has converged, U will be nearly equal to E , and hence the difference $U - E$ is a good criterion to guide the iteration process. A representative plot of $U - E$ as a function of K is shown in figure 5. The desired iteration point is obviously the first root of this function.

The first iteration is begun with $K = 50$, and the associated value of R' is found as outlined above; K is then increased in increments of 20, holding R fixed until $U \leq E$. Then, by interpolating to $U - E = 0$, a new value of K is found for the second iteration. A new value of R' is found from the new K value, which, in turn, leads to new values of U and E . The new values of U , E , and K , and the prior values of U , E , and K , are used to extrapolate to $U - E = 0$, which determines the next value of K . This process is continued until the value of K does not change during an iteration. K_{MAX} is then set equal to this value of K .

The iteration process is very fast, requiring only three or four iterations to converge to the maximum allowed value of K . K_{MAX} values computed in this manner for O_2 are in good agreement with the results of reference 10.

The maximum allowed rotational quantum number is found for both the upper and the lower vibrational levels. The value of K_{MAX} used in the program is the minimum of the upper state value, the lower state value, and the input value if one is specified. If the dissociation energy of an electronic level is not known, K_{MAX} cannot be found for that level. If K_{MAX} cannot be found for either level and a value is not input, the program arbitrarily sets $K_{MAX} = 150$; experience has found this to be a reasonable value except for the halides.

Constants Used in Rotational-Structure Subroutines

(a) Subroutine ZERO

The line-strength expression used for these transitions (i.e., $\Sigma \rightarrow \Sigma$, $\Pi \rightarrow \Pi$, etc.) is (see ref. 7)

$$S = KU + CSTR \quad (18)$$

where

$$\begin{aligned} CSTR &= 0 && \text{for the R branch} \\ CSTR &= 1 && \text{for the P branch} \end{aligned}$$

(b) Subroutine ONE

The line-strength expressions used for these transitions (i.e., $\Sigma \rightarrow \Pi$, $\Pi \rightarrow \Sigma$, $\Pi \rightarrow \Delta$, etc.) are (see ref. 7)

$$S(P) = \frac{(KU + 1 - \text{SIGN} \cdot \text{CAPLU})(KU + 2 - \text{SIGN} \cdot \text{CAPLU})}{2(KU + 1)} \quad (19)$$

$$S(Q) = \frac{(KU + \text{SIGN} \cdot \text{CAPLU})(2KU + 1)(KU + 1 - \text{SIGN} \cdot \text{CAPLU})}{2KU(KU + 1)} \quad (20)$$

$$S(R) = \frac{(KU + \text{SIGN} \cdot \text{CAPLU})(KU - 1 + \text{SIGN} \cdot \text{CAPLU})}{2KU} \quad (21)$$

For $\Delta\Lambda = +1$ transitions (i.e., $\Pi \rightarrow \Sigma$, $\Delta \rightarrow \Pi$, etc.)

$$\text{SIGN} = +1$$

For $\Delta\Lambda = -1$ transitions (i.e., $\Sigma \rightarrow \Pi$, $\Pi \rightarrow \Delta$, etc.)

$$\text{SIGN} = -1$$

(c) Subroutine S2 PI2

The wave number (NUBAR) of each rotational line for these transitions (i.e., $^2\Sigma \leftrightarrow ^2\Pi$) is defined by the equations in reference 9, page 232, or reference 7. In partial Fortran IV notation, the wave number is

$$\begin{aligned} \text{NUBAR} = & \text{NUBARO} + \text{BVU} \left[(\text{JU} + 0.5)^2 - \text{CAPLU}^2 \right. \\ & + \frac{\text{SIGNU1}}{2} \sqrt{4(\text{JU} + 0.5)^2 - 4 \cdot \text{YU} \cdot \text{CAPLU}^2 + (\text{YU} \cdot \text{CAPLU})^2} \\ & - \text{BVL} \left[(\text{JL} + 0.5)^2 - \text{CAPLL}^2 \right. \\ & \left. + \frac{\text{SIGNU2}}{2} \sqrt{4(\text{JL} + 0.5)^2 - 4 \cdot \text{YL} \cdot \text{CAPLL}^2 + (\text{YL} \cdot \text{CAPLL})^2} \right] \quad (22) \end{aligned}$$

The line-strength expression for each branch (see ref. 11, or ref. 7) is given by one of the following general expressions

$$S_1 = \frac{(2J + 1)^2 + \text{SIGNS1} \cdot (2J + 1) \cdot U \cdot (4J^2 + 4J + \text{CONST1} + 2Y \cdot \text{SIGNS2})}{16(J + \text{CONST2})} \quad (23)$$

$$S_2 = \frac{(2J+1)[(4J^2 + 4J - 1) - \text{SIGNS1} \cdot U \cdot (8J^3 + 12J^2 - 2J + \text{CONST3} + 2Y \cdot \text{SIGNS3})]}{16J(J+1)} \quad (24)$$

where

$$U = [Y^2 - 4Y + (2J+1)^2]^{-1/2} \quad (25)$$

$J = J_U$ and $Y = Y_U = \text{CAPAU}/\text{BVU}$ for $^2\Pi \rightarrow ^2\Sigma$ transitions

$J = J_L$ and $Y = Y_L = \text{CAPAL}/\text{BVL}$ for $^2\Sigma \rightarrow ^2\Pi$ transitions

The values of the constants in these expressions can be determined from references 9 and 11, and are tabulated in table I.

Integration in INTRVL and SLIT Subroutines

(a) Subroutine INTRVL

Subroutine INTRVL computes integrated intensities between the specified wavelengths LAM1 and LAM2. The integration is, simply,

$$\text{TOTALI} = \int_{\text{LAM1}}^{\text{LAM2}} \text{EIAM} \cdot d\lambda \quad (26)$$

A sketch to help clarify the notation used in the program is given in figure 6. The integration proceeds by assuming a linear variation of the spectral intensity between points in the array.

(b) Subroutine SLIT

Subroutine SLIT computes the output signal that would be recorded by an instrument measuring intensities equal to the computed spectrum. The instrument sensitivity is input by specifying the slit function and the absolute calibration. The slit function can be specified by a normalized Gaussian expression or by a series of linear segments. These two alternatives are illustrated in figure 7. In the case of a nonsymmetrical slit, as shown in figure 7(b), LAMCL is difficult to specify meaningfully. The width of the linear segment slit is defined as

$$\text{WIDTH} = \frac{\int \text{RSLIT} \cdot d\lambda}{\text{RMAX}} \quad (27)$$

The instrument absolute calibration is input as a single factor, if the instrument is a fixed wavelength radiometer, and as a function of wavelength, if the instrument is a grating spectrograph or a scanning spectrometer (referred to hereafter as a scanning slit). A representative calibration curve (RIAM(M)) for a scanning slit is shown in figure 8.

The integration to yield the instrument output signal at a given wavelength is

$$\text{SIGNAL} = \int \left(\begin{array}{c} \text{slit} \\ \text{function} \end{array} \right) \frac{\text{RSLIT} \cdot \text{RLAMCL} \cdot \text{ELAM}}{\text{C} \cdot \text{WIDTH}} d\lambda \quad (28)$$

where RLAMCL is either the calibration factor for a fixed wavelength slit or the local value of the calibration function for a scanning slit and,

C = 1.0 for a linear-segment slit function

C = 1.065 for a Gaussian slit function

The integration at a given wavelength is illustrated in figure 9. For a scanning slit, the integration is performed repetitively at wavelength intervals given by STEP from LAMS1 to LAMS2. Only 500 locations have been reserved in the computer for storing SIGNAL as a function of wavelength. However, after this storage is filled, the data are printed, permitting the storage to be used again for the next 500 points. Therefore, there is no limit to the number of instrument-output points that can be computed. The primary purpose of printing the data in 500 point blocks is to facilitate adding a machine-plotting option.

PROGRAM USAGE

The program is written in the Fortran IV computer language. It operates at Ames Research Center on an IBM 7094 computer as an overlay job, under the IBJOB Processor of the IBSYS Operating System, version 13.

A simplified flow chart of the main program, illustrating the step-by-step flow through the program, is shown in figure 1. The primary method used to control the sequence of operations is the presence or absence of data in various fields of certain data cards. The inset table in figure 1 lists the data cards that are tested and the data fields that are filled for each card type. Clearly, by testing for blanks (or zeros), the card type can be selected. At the end of each case, control is transferred back to the beginning of the program to read in the next case. There is no limit to the number of cases that can be "stacked."

Deck Makeup

<u>Origin</u>	<u>Link</u>	<u>Name</u>	<u>Description</u>
---	0	MAIN	Initializes factors for each case, directs logic to the appropriate subroutines, and solves the radiative-transport equation
---	0	BLOCK DATA	Fills array OUTPUT
---	0	SKIP	Positions data tape to start of desired file. User must provide this subroutine. (When called from SETUP it skips to the start of the next file, when called from VU VL it returns to the start of the present file.)
ALPHA	1	ILAMDA	Initializes the ILAM array with the specified incident radiation and initializes the ELAM array to 0.0
ALPHA	2	SETUP	Reads the molecular constants, computes the partition function, and determines the appropriate transition subroutine to generate the intensities
ALPHA	3	VU VL	Computes and reads vibrational band constants, determines the maximum rotational quantum number, and finds the intensity factor
ALPHA	4	ZERO	Computes parallel transitions for diatomic molecules
ALPHA	5	ONE	Computes perpendicular transitions for diatomic molecules
ALPHA	6	S2 PI2	Computes doublet sigma to doublet pi transitions (or vice versa) for diatomic molecules
ALPHA	7	ATOMIC	Computes the electronic transitions for atoms
ALPHA	8	PRINT	Tabulates spectral intensity vs. wavelength on the written output
ALPHA	9	INTRVL	Computes integrated intensities between specified wavelengths
ALPHA	10	SLIT	Computes the output signal given by a specified instrument sensitivity
ALPHA	11	GROWTH	Computes the curve-of-growth

Tapes

<u>Logical tape number</u>	<u>Usage</u>
5	Input
6	Output
9	Spectroscopic data tape. BCD format, 800 bits/inch.

Program Input

A complete description of all required data cards is given in appendix C. Clearly, for the program to function properly, a great many values must be specified correctly. To reduce the probability of costly human errors, the spectroscopic constants and Franck-Condon factors for 18 diatomic band systems are stored on magnetic tape. A listing of this tape is given in appendix D. The tape can be easily extended to include additional band systems.

The program logic is such that all spectroscopic constants for a given band system must be read from the tape, or all must be read from data cards. If the spectroscopic constants are read from the tape, then the Franck-Condon factors may also be read from the tape. However, because Franck-Condon factors are generally more uncertain than the spectroscopic constants, the option exists to override the Franck-Condon factor on the tape by specifying the desired value on the appropriate data card.

Computer Run Time

The time to run a single case on the computer is controlled primarily by the time required to generate the spontaneous-emission spectrum. Therefore, the computer run time can be estimated approximately by

$$\text{Time} = c \cdot n \cdot \text{RANGE} \cdot (\text{WIDTHV} / \text{DELLAM}), \text{ minutes} \quad (29)$$

where

c constant found from experience with a given computer,
 5.8×10^{-5} minute/line for the ARC IBM 7094

n total number of lines included in the computation

Error Flags

Tests are made at many strategic locations throughout the program to insure that obvious errors are not present in the data. If an obvious error is found, an appropriate statement is printed. If an error is found in the data for the externally incident radiation, the program skips to the next case. If an error is found in the data for a band system, the program transfers control to the PRINT subroutine, which prints, in tabular form, the spectrum computed to that point, and then skips to the next case. If an error is found in the data for a vibrational band, an appropriate statement is printed, and the band is omitted from the calculation. However, in this case, the solution will continue.

Sample Case

The sample case presented is intended to illustrate the general format of the printed output. Therefore, only a few of the program options are included. A complete checkout of all program options and error flag statements has been made, but such an extensive checkout does not seem appropriate for this report. The sample case selected for presentation is the CN(red) and atomic-nitrogen computation shown in figures 7(a) and 7(b) of reference 7. The printed output for this case is shown in appendix E. Considerable care has been taken to output all input data used in the computation and to clearly identify each of them. Standard spectroscopic nomenclature from reference 9 has been used where appropriate. Where this was not possible, more complete statements have been printed.

The heading on the printed output is composed of the information placed on the three title cards plus a statement of the spectral range of the computation and the wavelength interval between computation points. Following the heading, each molecular band system and atomic system specified is printed. The spectroscopic constants and thermodynamic conditions specified for each system are also printed, in addition to the computed values of the spontaneous-emission intensity.

The integrated intensity listed for each branch is the sum of the spontaneous emission from all rotational lines between KMIN and KMAX that fall within the spectral range of the computation. BAND TOTAL is simply the sum of the branch intensities. APPROXIMATE BAND TOTAL is computed by assuming that all the band radiation occurs at the band origin (see equation IV-74 on page 200 of reference 9) and is normally within 30 percent or less of the BAND TOTAL. A larger difference is shown here because most of the rotational lines fall outside the spectral range specified and, therefore, are not included in the BRANCH and BAND TOTAL values. After the vibrational bands specified for a band system have been computed, the integrated spontaneous emission from the entire system, SYSTEM TOTAL, is found by summing the BAND TOTAL values. In the sample case, only one band is specified so that SYSTEM TOTAL = BAND TOTAL. The output for the atomic-nitrogen lines illustrates a format similar to, but somewhat simpler than, that for the band systems. After the last molecular or atomic system has been completed, the sum of the integrated spontaneous emission from every rotational and atomic line that fell within the spectral range is printed.

Once the computation of the spontaneous-emission spectrum is complete, for a case or a layer, cards are read that specify whether an optically thin spectrum is desired, or whether the "true" spectrum given by the equation of radiative transfer is desired (see discussion in ref. 7). For this sample case, a "true" spectrum is specified for a radiating gas depth of 1.0 cm, and it is tabulated on the printed output. Only a partial tabulation is presented.

The final program option illustrated by this sample case is the spectrum as it would appear if recorded by a grating instrument. The slit function and spectral calibration assumed for the calculation are shown on the printed output, and in figure 7(b) of reference 7. The instrument sensitivity at any

wavelength is given by the product of these functions. The instrument output signal is found by integrating the product of the instrument sensitivity and the spectral intensity. A partial tabulation of the output signal as a function of wavelength is shown on the printed output, and can be compared with figure 7(a) of reference 7.

CONCLUDING REMARKS

The computer program presented is applicable, to some degree of approximation, to any "allowed" diatomic or atomic electronic transition. The program computes a "true" spectrum by using the equation of radiative transfer, which accounts for spontaneous emission, induced emission, absorption, and externally incident radiation. Considerable care has been taken to make the program easy to read and apply. Since standard spectroscopic notation is used and abundant comment statements are provided within the actual program listing, the user should be able to understand the program and not be forced to exhibit faith in a "canned" routine. In addition, the program was designed to enable additional subroutines to be added with only minor modifications to the main program. Likely candidates for addition to the program are subroutines to compute the free-free and free-bound continua.

Ames Research Center

National Aeronautics and Space Administration

Moffett Field, Calif., 94035, Dec. 2, 1968

124-07 -01-15-00-21

APPENDIX A

LISTING OF PROGRAM STATEMENTS

```

$JOB  DEBUG  ARNOLD  HF0750R2812  20000  4.0  2821  SEPT 19, 68
$IBJOB  BASIC
$DECK  DUM03
$DECK  DUM04
$DECK  DUM07
$DECK  DUM08
$DECK  DUM10
$DECK  DUM11
$DECK  DUM12
$IBFTC  HF0750

```

19

C MAIN PROGRAM

C INITIALIZES FACTORS FOR EACH CASE, DIRECTS LOGIC TO THE APPROPRIATE
C SUBROUTINES, AND SOLVES THE RADIATIVE TRANSPORT EQUATION.

```

COMMON/CPL0T/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/ILAM( 9000),ELAM( 9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
1  ALPHA,BEL,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL,TERML
COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,MU,ALTNAT,
1  WEL,WEXEL,WEYEL,WEZEL,BVL,DVL, NUSPIN
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
COMMON/CTRAN/PARTCC,NUBARO,Q,AOE,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

DIMENSION TITLE(36)
REAL ILAM,LAMMAX,LAMMIN,MU,NUBARO,NUSPIN,LAMBDA
LOGICAL NEWCAS
DATA BLANK/6H      /, PRINTS/6HPRINT /, CASE/4HCASE/

```

C-----

C READ THE FIRST CONTROL CARD IN EACH CASE. IF FIRST 4 COLUMNS DO NOT SPELL
C CASE, READ THROUGH TO THE NEXT CASE.

```

10  READ (5,505) SEARCH
    IF (SEARCH .EQ. CASE) GO TO 20
    GO TO 10

```

C INITIALIZE RUNNING SUMS, CONSTANTS, AND FLAGS FOR THE NEW CASE.

```

20  TOTAL=0.0
    SYSTEM=0.0
    DEPTH=0.0
    CINT3=0.0
    DO 30 M=1,5

```

C OUTPUT(11) IS A BLANK CHARACTER SET IN BLOCK DATA.

```

30  FACTRI(M)=OUTPUT(11)

    NEWCAS= .FALSE.

```

C READ TITLE CARDS FOR THIS CASE.

```

    READ(5,500) (TITLE(M),M=1,36)

```

C PRINT TITLES ON WRITTEN OUTPUT.

```

    WRITE(6,600) (TITLE(M),M=1,36)

```

C READ WAVELENGTH RANGE FOR CALCULATION AND WAVELENGTH INTERVAL BETWEEN
C POINTS IN THE COMPUTED SPECTRUM.

```

    READ(5,501) LAMMIN,LAMMAX,DELLAM

```

C TEST DELLAM. IF IT IS TOO SMALL TO ALLOW COVERAGE FROM LAMMIN TO
C LAMMAX WITH 9,000 ENTRIES IN THE ARRAY, INCREASE DELLAM.

```

    IF ((LAMMAX-LAMMIN)/DELLAM.GT. 8999.) DELLAM=(LAMMAX-LAMMIN)/8999.
    NARRAY=1.1 +(LAMMAX-LAMMIN)/DELLAM

```

C ADJUST LAMMAX TO MAKE IT AN EVEN INCREMENT OF DELLAM AND WRITE GENERAL
C HEADING FOR THIS CASE.

```

    ARRAYN=NARRAY
    LAMMAX=LAMMIN +(ARRAYN-1.0)*DELLAM
    WRITE(6,602) LAMMIN,LAMMAX,DELLAM

```

C SUBROUTINE ILAMDA INITIALIZES THE ILAM ARRAY WITH THE SPECIFIED
C INCIDENT RADIATION AND INITIALIZES THE ELAM ARRAY TO 0.0.
C IF NEWCAS = .TRUE., AN ERROR WAS DETECTED IN THE INCIDENT SPECTRUM
C AND THIS CASE WILL BE OMITTED.

```

    CALL ILAMDA (NEWCAS)
    IF (NEWCAS) GO TO 10
    GO TO 50

```

C-----

C STATEMENT 40 IS A KEY READ STATEMENT IN THE PROGRAM. REQUIRED
C INFORMATION IS READ AND THE PROGRAM TESTS WHICH FIELDS HAVE DATA
C TO DETERMINE WHAT SHOULD BE DONE NEXT. WHEN RETURNING FROM THE
C ILAMDA OR ATOMIC SUBROUTINES, THIS CARD HAS ALREADY BEEN READ.

C THE FOLLOWING TABLE DEFINES THE FIELDS THAT ARE FILLED FOR
C EACH CARD TYPE.

C CARD TYPE	READ1	READ2	READ3	READ4	READ5	READ6
C (COLUMNS)	1-10	11-20	21-30	31-40	41-45	67-72
C (TYPE FIELD)	E10.0	E10.0	E10.0	E10.0	F5.0	A6

C VIBRATIONAL BAND	VU	VL	KMIN	KMAX		
C BAND						
C SYSTEM	PARTCC	TELECT	TVIB	TROT	(IF ON CARDS) (INDEX)	NAME
C ATOMIC SYSTEM	ATOMCC	TELECT	PARTITION FUNCTION-Q			NAME
C CURVE OF GROWTH	LAM1	LAM2				GROWTH
C RADIATIVE TRANSPORT	DEPTH					LAYER
C PRINT SPECTRUM						PRINT
C DONT PRINT SPECTRUM						NONE


```

40 READ(5,502) READ1,READ2,READ3,READ4,READ5,READ6
C WHAT CARD TYPE HAS BEEN READ.
C IS THIS A VIBRATIONAL BAND.
50 IF(READ6 .EQ. BLANK) GO TO 70
C IS THIS A BAND SYSTEM.
    IF (READ4 .NE. 0.0) GO TO 60
C IS THIS AN ATOMIC SYSTEM.
    IF (READ3 .NE. 0.0) GO TO 110
C THE SPONTANEOUS EMISSION SPECTRUM FOR THIS CASE OR LAYER IS COMPLETE.
    TOTAL=TOTAL+SYSTEM
    IF (TOTAL .EQ. 0.0) GO TO 55
    IF (SYSTEM .NE. 0.0) WRITE(6,606) SYSTEM,(FACTRI(M),M=1,5)
    WRITE(6,607) TOTAL,(FACTRI(M),M=1,5)
    SYSTEM= 0.0
    TOTAL= 0.0
C IS THIS A CURVE OF GROWTH CALCULATION.
55 IF (READ2 .NE. 0.0) GO TO 115
C IS THIS A RADIATIVE TRANSPORT CALCULATION.
    IF (READ1 .NE. 0.0) GO TO 120
    GO TO 160
C-----
C TRANSFER CONTROL TO THE APPROPRIATE SUBROUTINE.
C SUBROUTINE SETUP READS THE MOLECULAR CONSTANTS, COMPUTES THE PARTITION
C FUNCTION, AND DETERMINES THE APPROPRIATE TRANSITION SUBROUTINE TO
C GENERATE INTENSITIES DUE TO SPONTANEOUS EMISSION. IF NEWCAS = .TRUE. AN ERROR
C WAS DETECTED IN THE MOLECULAR CONSTANTS AND THE REMAINDER OF THIS
C CASE WILL BE OMITTED.
60 CALL SETUP (NEWCAS)
    IF (NEWCAS) GO TO 180
    GO TO 40
C SUBROUTINE VU VL COMPUTES AND READS VIBRATIONAL BAND CONSTANTS
C AND DETERMINES THE MAXIMUM ROTATIONAL QUANTUM NUMBER AND THE INTENSITY
C FACTOR.
70 CALL VU VL (SKIPVV)
    IF (SKIPVV .NE. 0.0) GO TO 40
    GO TO (80,90,100),INDEX
C SUBROUTINE ZERO COMPUTES PARALLEL TRANSITIONS FOR DIATOMIC MOLECULES.
80 CALL ZERO
    GO TO 40
C SUBROUTINE ONE COMPUTES PERPENDICULAR TRANSITIONS FOR
C DIATOMIC MOLECULES.
90 CALL ONE
    GO TO 40
C SUBROUTINE S2 PI2 COMPUTES DOUBLET SIGMA TO DOUBLET PI TRANSITIONS
C (OR VICE VERSA) FOR DIATOMIC MOLECULES.
100 CALL S2PI2
    GO TO 40
C SUBROUTINE ATOMIC COMPUTES ELECTRONIC TRANSITIONS FOR ATOMS.

```

```

110 CALL ATOMIC
    GO TO 50

C THIS IS A CURVE-OF-GROWTH CALCULATION.

115 CALL GROWTH
    DEPTH= 0.0

C RE-INITIALIZE THE ILAM ARRAY TO ENABLE A SEPARATE RADIATIVE TRANSPORT
C CALCULATION IF SPECIFIED.

    DO 117 M=1,NARRAY
117   ILAM(M)=0.0
    GO TO 40

C-----
C THIS IS A RADIATIVE TRANSPORT SOLUTION. GENERATE THE ILAM ARRAY.

120 DEPTH =READ1
    WRITE(6,608) DEPTH
    DO 130 M=1,NARRAY
        IF(ELAM(M) .LE. 1.0E-36) GO TO 130
        COUNT=M
        LAMBDA=(LAMMIN +(COUNT-1.0)*DELLAM)*1.0E-8
        BLAM=1.1904E-16*EXP(-1.43879/(LAMBDA*TELECT))/(LAMBDA**5*
1      (1.0-EXP(-1.43879/(LAMBDA*TELECT))))
        CILAM1=ALOG(8.40032E+15*LAMBDA**5*(1.0-EXP(-1.43879/
1      (LAMBDA*TELECT))))
        CILAM2=ALOG(DEPTH)
        CILAM3=ALOG(ELAM(M))
        CILAM4=1.43879/(LAMBDA*TELECT)-2.30259*CINT3+CILAM1+CILAM2

        1      +CILAM3
        IF (CILAM4 .GT. 87.0) CILAM4=87.0
        CILAM4=EXP(CILAM4)
        ILAM(M)=BLAM-(BLAM-ILAM(M))*EXP(-CILAM4)
130    CONTINUE

C THE ILAM ARRAY HAS BEEN GENERATED FOR THIS LAYER.
C INITIALIZE THE INTENSITY FACTOR AND ELAM ARRAY FOR THE NEXT LAYER.

    CINT3=0.0
    DO 140 M=1,5
140    FACTRI(M)= OUTPUT(11)

    DO 150 M=1,NARRAY
150    ELAM(M)=0.0
    GO TO 40

C-----
C THE CALCULATION OF THE FINAL SPECTRAL INTENSITY ARRAY IS FINISHED.
C COMPLETE THE SOLUTION FOR THE OUTPUT OPTIONS DESIRED.
C IF THIS IS A RADIATIVE TRANSPORT SOLUTION, TRANSFER THE VALUES OF
C ILAM INTO THE ELAM ARRAY FOR CONVENIENCE IN LATER MANIPULATION.

160 IF(DEPTH .EQ. 0.0) GO TO 180
    DO 170 M=1,NARRAY
170    ELAM(M)=ILAM(M)

C GENERATE WAVELENGTHS AND STORE THEM IN THE ILAM ARRAY.

180 DO 190 M=1,NARRAY
    COUNT=M
190    ILAM(M)=LAMMIN +(COUNT-1.0)*DELLAM

    IF (NEWCAS) GO TO 200

C IS THE SPECTRUM TO BE TABULATED.

    IF(READ6 .NE. PRINTS) GO TO 210

C SUBROUTINE PRINT TABULATES SPECTRAL INTENSITY VERSUS WAVELENGTH ON
C THE WRITTEN OUTPUT.

200 CALL PRINT(NEWCAS)
    IF (NEWCAS) GO TO 10

C READ A CARD WHICH SPECIFIES THE NUMBER OF INTERVALS AND THE NUMBER
C OF SLITS TO BE CONSIDERED.

210 READ(5,503) NINTRV,NSLIT

C SUBROUTINE INTRVL COMPUTES INTEGRATED INTENSITIES BETWEEN SPECIFIED
C WAVELENGTHS.

    IF (NINTRV .NE. 0) CALL INTRVL(NINTRV)

C SUBROUTINE SLIT COMPUTES THE OUTPUT SIGNAL GIVEN BY A SPECIFIED
C INSTRUMENT SENSITIVITY.

    IF (NSLIT .NE. 0) CALL SLIT(NSLIT)
    GO TO 10

C-----
C FORMATS FOR READ STATEMENTS.

```

```

500  FORMAT(12A6)
501  FORMAT(3E10.0)
502  FORMAT(4E10.0,F5.0,21X,A6)
503  FORMAT(215)
504  FORMAT(4E10.3,26X,A6)
505  FORMAT(1A4)

```

C FORMATS FOR WRITE STATEMENTS.

```

600  FORMAT(1H1,29X,12A6/30X,12A6/30X,12A6)
601  FORMAT(31X,12A6)
602  FORMAT(/21X,27HTHE SPECTRUM COMPUTED FROM ,F8.2,4H TO ,F8.2,
1    14H ANGSTROMS AT ,F6.3,19H ANGSTROM INTERVALS//)
606  FORMAT(103X,12HSYSTEM TOTAL,1X,1PE10.4,5A1)
607  FORMAT(/80X,35HTOTAL OF ALL INTEGRATED INTENSITIES,1X,1PE10.4,5A1)
608  FORMAT(/24X,73HTHIS IS A RADIATIVE TRANSPORT SOLUTION, DEPTH OF A
    ABOVE RADIATING LAYER IS,F9.3,4H CM.//)

```

END

\$IBFTC HF075A

BLOCK DATA

C BLOCK DATA SUBROUTINE IS USED TO LOAD HOLLERITH INFORMATION INTO THE
C ARRAY, OUTPUT(12). THIS ARRAY IS USED TO BUILD THE ARRAY FACTRI(5)
C FOR PRINTING THE INTENSITY FACTOR.

COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

```

DATA (OUTPUT(M),M=1,12)/1H0,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9,
1    1H ,1H-/

```

END

\$IBFTC HF075N

SUBROUTINE SKIP(1,K)

C SUBROUTINE SKIP POSITIONS THE SPECTROSCOPIC DATA TAPE (TAPE 9) TO THE
C PROPER FILE.

WRITE (6,700)

STOP

C FORMAT FOR ERROR STATEMENT.

```

700  FORMAT(/30X,48HTHE COMPUTATION WAS TERMINATED BECAUSE THE USER ,
1    23HHAS NOT SUPPLIED A SKIP/
2    30X,46HSUBROUTINE TO POSITION THE SPECTROSCOPIC DATA ,
3    24HTAPE TO THE PROPER FILE.//)

```

END

\$ORIGIN ALPHA
\$IBFTC HF075B

SUBROUTINE ILAMDA (NEWCAS)

C SUBROUTINE ILAMDA INITIALIZES THE ILAM ARRAY WITH THE SPECIFIED
C INCIDENT RADIATION AND INITIALIZES THE ELAM ARRAY TO 0.0.

```

COMMON/CPLT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/ILAM( 9000),ELAM( 9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU
1    ALPHAL,BEL,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL,TERML
COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,MU,ALTNAT,
1    WEL,WEXEL,WEYEL,WEZEL,BVL,DVL, NUSPIN
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
COMMON/CTRAN/PARTCC,NUBARO,Q,A0E,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

```

```

REAL ILAM,LAMMAX,LAMMIN
LOGICAL NEWCAS
DATA BLANK/6H

```

C INITIALIZE VALUES SO THAT THE ILAM ARRAY CAN BE SET TO 0.0 IF AN INCIDENT
C SPECTRUM IS NOT SPECIFIED.

```

ELAM(1)=LAMMIN
ELAM(2)=LAMMAX

```

```

ELAM(5001)=0.0
ELAM(5002)=0.0

```

```

NLAM=-1
NILAM=4999
NOILAM= 0

```

C READ THE VALUES OF THE INCIDENT RADIATION VERSUS WAVELENGTH AND STORE
C THEM TEMPORARILY IN THE ELAM ARRAY.

```

10  READ(5,500) READ1,READ2,READ3,READ4,READ5,READ6
    IF(READ6 .NE. BLANK) GO TO 20
    NOILAM= 1
    NLAM=NLAM+2
    NILAM=NILAM+2
    ELAM(NLAM)=READ1
    ELAM(NILAM)=READ2
    ELAM(NLAM+1)=READ3
    ELAM(NILAM+1)=READ4
    GO TO 10

20  NLAM=NLAM+1
    IF(NLAM.NE.0) GO TO 25
    M1=1
    GO TO 50

25  IF (ELAM(NLAM) .EQ. 0.0) NLAM=NLAM-1

C  PRINT SPECIFIED INCIDENT RADIATION.

    WRITE(6,600)
    DO 30 M=1,NLAM
30  WRITE(6,601) ELAM(M),ELAM(M+5000)

C  TEST WAVELENGTHS OF THE INITIAL ILAM VALUES.

C  THE LAST WAVELENGTH MUST BE EQUAL TO OR GREATER THAN LAMMAX.
C  THE FIRST WAVELENGTH MUST BE LESS THAN OR EQUAL TO LAMMIN.
C  SET THE INDEX M1 SO THAT LAMMIN IS BOUNDED BY THE APPROPRIATE ELAM ELEMENTS.
C  WAVELENGTHS MUST INCREASE MONOTONICALLY.

    IF(ELAM(NLAM) .LT. LAMMAX) GO TO 80
    M1=0
35  IF(ELAM(M1+1) .GT. LAMMIN) GO TO 38
    M1=M1+1
    GO TO 35
38  IF(M1 .EQ. 0) GO TO 80
    DO 40 M=2,NLAM
        IF (ELAM(M) .LE. ELAM(M-1)) GO TO 80
40  CONTINUE

C  INITIALIZE THE ILAM ARRAY.

50  DO 60 M=1,NARRAY
    COUNT=M
    ILAM(M)=ELAM(M1+5000) +(ELAM(M1+5001)-ELAM(M1+5000))*(LAMMIN+
1  (COUNT-1.0)*DELLAM-ELAM(M1))/(ELAM(M1+1)-ELAM(M1))
60  IF (LAMMIN+COUNT*DELLAM .GT. ELAM(M1+1)) M1=M1+1

C  INITIALIZE THE ELAM ARRAY.

    DO 70 M=1,NARRAY
70  ELAM(M)=0.0
    RETURN

C  THERE IS AN ERROR IN THE INCIDENT RADIATION DATA. WRITE
C  AN ERROR MESSAGE AND OMIT THIS CASE.

80  WRITE(6,700)
    NEWCAS=.TRUE.
    RETURN

C  FORMATS FOR READ STATEMENTS.

500  FORMAT(4E10.0,F5.0,21X,A6)

C  FORMATS FOR WRITE STATEMENTS.

600  FORMAT(48X,35HSPECTRUM INCIDENT ON GAS SAMPLE//
1  51X,10HWAVELENGTH,10X,8HINCIDENT/
2  51X,2HIN,18X,9HINTENSITY/
3  51X,9HANGSTROMS,11X,15HW/CM2-MICRON-SR//)
601  FORMAT(50X,F8.2,13X,1PE10.4)

C  FORMAT FOR ERROR STATEMENT.

700  FORMAT(/22X,50HONE OF THE FOLLOWING RESTRICTIONS ON THE INCIDENT
1  ,37HSPECTRAL INTENSITY ARRAY WAS VIOLATED/
2  36X,58HTHE FIRST WAVELENGTH MUST BE LESS THAN OR EQUAL TO L
3  AMMIN./
4  36X,60HTHE LAST WAVELENGTH MUST BE EQUAL TO OR GREATER THAN
5  LAMMAX./
6  36X,40HWAVELENGTHS MUST INCREASE MONOTONICALLY.)

    END
*****

```

SORIGIN ALPHA
\$IBFTC HF075C

SUBROUTINE SETUP (NEWCAS)

C SUBROUTINE SETUP READS THE MOLECULAR CONSTANTS, COMPUTES THE PARTITION
C FUNCTION, AND DETERMINES THE APPROPRIATE TRANSITION SUBROUTINE TO
C GENERATE INTENSITIES DUE TO SPONTANEOUS EMISSION.

```
COMMON/CPLLOT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/ILAM( 9000),ELAM( 9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
1 ALPHA,BEL,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL,TERML
COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,MU,ALTNAT,
1 WEL,WEXEL,WEYEL,WEZEL,BVL,DVL, NUSPIN
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
COMMON/CTRAN/PARTCC,NUBARO,Q,A0E,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)
```

```
DIMENSION ALPHA(30),BE(30),DEGEN(30),TERM(30),WE(30),
1 WEXE(30),WEYE(30),WEZE(30),DUMMY(2)
REAL KMAX1,KMAX2,LOWER,MU,NUBARO,NUSPIN,ILAM,NAME
LOGICAL NEWCAS
DATA ENDS/6HEND /, BLANK/6H /
DATA UPPER/6HUPPER /, LOWER/6HLOWER /, STATE/6HSTATE /
DATA ODD/6H ODD /, EVEN/6H EVEN /
```

REWIND 9

C A NEW BAND SYSTEM HAS BEEN SPECIFIED.

```
PARTCC=READ1
TELECT=READ2
TVIB=READ3
TROT=READ4
INDEX=READ5+.1
```

C WRITE THE INTEGRATED INTENSITY DUE TO SPONTANEOUS EMISSION FOR THE
C PREVIOUSLY COMPUTED SYSTEM.

```
IF (SYSTEM.NE. 0.0) WRITE(6,600) SYSTEM,(FACTRI(M),M=1,5)
TOTAL=TOTAL+SYSTEM
SYSTEM=0.0
```

C ARE THE CONSTANTS FOR THIS BAND SYSTEM INPUT ON CARDS.

```
IF (INDEX.NE. 0) GO TO 40
```

C THE CONSTANTS FOR THIS BAND SYSTEM ARE ON TAPE.

```
10 READ(9,900) NAME, INDEX, NFILE
IF (NAME.EQ. ENDS) GO TO 120
IF (NAME.EQ. READ6) GO TO 20
CALL SKIP(1,9)
GO TO 10
```

C READ PAST THE FRANCK-CONDON FACTORS, USING TERM(M2) AS A DUMMY
C ARRAY.

```
20 DO 30 M1=1,20
30 READ(9,901) (TERM(M2), M2= 1,20)
```

C READ THE CONSTANTS FROM TAPE.

```
READ (9,902) READ1,ALTNAT,DEU,BETAU,REU,DZEROU,CAPAU,CAPLU,
1 MU,NUSPIN,DEL,BETAL,REL,DZEROL,CAPAL,CAPLL
LEVELS=READ1+0.1
READ (9,902) (DEGEN(M),TERM(M),WE(M),WEXE(M),WEYE(M),WEZE(M),BE(M),
1 ALPHA(M),M=1,LEVELS)
GO TO 50
```

C THE CONSTANTS FOR THIS BAND SYSTEM ARE TO BE INPUT ON CARDS.

```
40 READ(5,500) READ1,ALTNAT,DEU,BETAU,REU,DZEROU,CAPAU,CAPLU
READ(5,500) MU,NUSPIN,DEL,BETAL,REL,DZEROL,CAPAL,CAPLL
LEVELS=READ1+0.1
READ(5,500) (DEGEN(M),TERM(M),WE(M),WEXE(M),WEYE(M),WEZE(M),
1 BE(M),ALPHA(M),M=1,LEVELS)
NFILE= 0
```

C STORE UPPER AND LOWER STATE SPECTROSCOPIC CONSTANTS FOR THIS SYSTEM.

```
50 ALPHAU=ALPHA(1)
ALPHA=ALPHA(2)
BEU=BE(1)
BEL=BE(2)
DEGENU=DEGEN(1)
TERMU=TERM(1)
TERML=TERM(2)
WEU=WE(1)
WEL=WE(2)
WEXEU=WEXE(1)
WEXEL=WEXE(2)
WEYEU=WEYE(1)
WEYEL=WEYE(2)
WEZEU=WEZE(1)
WEZEL=WEZE(2)
```

```

C FIND Q, THE PARTITION FUNCTION REFERENCED TO THE EQUILIBRIUM POSITION
C OF THE GROUND STATE POTENTIAL WELL.

      Q=0.0
      DO 70 M=1,LEVELS
        QVR=0.0
        QV=0.0
        EVIB1=0.0
        V=0.0
60      1 EVIB2=WE(M)*(V+0.5) -WEZE(M)*(V+0.5)**2 +WEYE(M)*(V+0.5)**3
          +WEZE(M)*(V+0.5)**4
          DELTQV=EXP(-1.43879*EVIB2/TVIB)

C COMPARE DELTA Q-VIBRATIONAL TO 0.1 PERCENT OF THE QV SUM TO THIS
C POINT.

          IF (DELTQV .LE. 0.001*QV) GO TO 70

C HAS THE VIBRATIONAL ENERGY REACHED A FICTITIOUS PEAK.

          IF (EVIB2 .LE. EVIB1) GO TO 70

          QV=QV+DELTQV
          QVR=QVR +TROT*DELTQV/(1.43879*(BE(M)-ALPHA(M)*(V+0.5)))
          EVIB1=EVIB2
          V=V+1.0
          GO TO 60
70      Q=Q +QVR*DEGEN(M)*EXP(-1.43879*TERM(M)/TELECT)

C WRITE THE INPUT DATA FOR THE NEW SYSTEM.

      WRITE(6,601) READ6,PARTCC,TELECT,TVIB,TROT
      WRITE(6,602) ALTNAT,NUSPIN,LEVELS,MU

      ICAPLU= CAPLU+ 0.1
      ICAPLL= CAPLL+ 0.1
      WRITE(6,606)CAPAU,ICAPLU,DEU,BETAU,DZEROU,REU,
1      CAPAL,ICAPLL,DEL,BETAL,DZEROL,REL
      WRITE(6,607)

      DO 100 M=1,LEVELS
        DUMMY(1)=BLANK
        DUMMY(2)=BLANK
        IF (M .NE. 1) GO TO 80
        DUMMY(1)= UPPER
        DUMMY(2)= STATE
80      IF (M .NE. 2) GO TO 90
        DUMMY(1)= LOWER
        DUMMY(2)= STATE
90      MDUMMY = DEGEN(M)
100     1 WRITE(6,603) DUMMY(1),DUMMY(2),MDUMMY,TERM(M),WE(M),WEZE(M),
          WEYE(M),WEZE(M),BE(M),ALPHA(M)

C IF LINES ALTERNATE IN INTENSITY, WRITE OUT RATIO OF INTENSITIES.

      IF (ALTNAT .EQ. 0.0) GO TO 110
      DUMMY1=ODD
      IF (ALTNAT .EQ. 2.0) DUMMY1=EVEN
      RATIO=NUSPIN/(NUSPIN+1.0)
      WRITE(6,604) DUMMY1,RATIO

C IS THE UPPER ELECTRONIC TERM ENERGY GREATER THAN THE LOWER ELECTRONIC
C TERM ENERGY. IF NOT, WRITE AN ERROR MESSAGE AND OMIT THIS CASE.

110    IF (TERMU .LE. TERML) GO TO 130

C WRITE THE OUTPUT HEADING FOR VIBRATIONAL BANDS.

      WRITE(6,605)
      RETURN

C THERE IS AN ERROR IN THE BAND SYSTEM NAME. WRITE AN ERROR MESSAGE
C AND OMIT THIS CASE.

120    WRITE(6,700) READ6
      GO TO 140

C THERE IS AN ERROR IN THE TERM ENERGIES. WRITE AN ERROR MESSAGE AND
C OMIT THIS CASE.

130    WRITE(6,701)
140    NEWCAS=.TRUE.
      RETURN

C FORMATS FOR READ STATEMENTS.

500    FORMAT(8E10.0)
501    FORMAT(4E10.0,F5.0,21X,A6)
502    FORMAT(215)

C FORMATS FOR WRITE STATEMENTS.

600    FORMAT( /102X,12HSYSTEM TOTAL,2X,1PE10.4,5A1)
601    FORMAT(//63X,A6///
1      21X,12HTOTAL NUMBER,13X,10HELECTRONIC,14X,11HVIBRATIONAL,13X,
2      10HROTATIONAL/
3      21X,12HOF MOLECULES,3(13X,11HTEMPERATURE)/
4      21X,7HPER CC ,3X,3(15X,9HDEGREES K)//
5      21X,1PE10.4,1X,3(14X,E10.4)///)

```

```

602  FORMAT(21X,4HLINE,21X,12HNUCLEAR SPIN,12X,9HNUMBER OF,15X,
1    7HREDUCED/
2    21X,11HALTERNATION,14X,15HFOR HOMONUCLEAR,9X,
3    10HELECTRONIC,14X,6HATOMIC/
4    21X,6HFACTOR,19X,9HMOLECULES,15X,6HLEVELS,18X,6HWEIGHT//
5    23X,F2.0,24X,F3.1,21X,I2,19X,F6.4////)
603  FORMAT(1X,2A6,2X,I2,7X,7(1X,1PE14.7))
604  FORMAT(/6X,10HLINES WITH,A6,84HROTATIONAL QUANTUM NUMBERS ARE STR
1    LONGEST, WITH THE RATIO OF WEAK TO STRONG LINES OF ,F7.3)
605  FORMAT(/1X,11HVIBRATIONAL,3X,7HFRANCK-,6X,17HTRANSITION MOMENT,
1    3X,15HROTATIONAL LINE,10X,5HRANGE,7X,4HBAND,9X,
2    10HROTATIONAL,8X,10HINTEGRATED/
3    1X,11HQUANTUM NO.,3X,6HCONDON,7X,17HAVERAGED OVER THE,3X,
4    20HWIDTH AT HALF-HEIGHT,5X,7HIN LINE,5X,9HORIGIN IN,4X,
5    15HQUANTUM NUMBERS,3X,9HINTENSITY/
6    1X,11HUPPER LOWER,3X,6HFACTOR,7X,15HELECTRONIC BAND,5X,
7    21HGAUSS LORENTZ VOIGT,4X,6HWIDTHS,6X,9HANGSTROMS,6X,
8    11HMIN MAX,5X,8HW/CM2-SR)
606  FORMAT(14X,4HSPIN,9X,17HQUANTUM NUMBER OF,15X,10HROTATIONAL,5X,
1    10HROTATIONAL,7X,12HDISSOCIATION,5X,
2    21HINTERNUCLEAR DISTANCE/
3    14X,8HCOUPLING,5X,28HRESULTANT ELECTRONIC ANGULAR,4X,
4    8HCONSTANT,7X,8HCONSTANT,9X,6HENERGY,11X,14HAT EQUILIBRIUM/
5    14X,8HCONSTANT,5X,29HMOMENTUM ABOUT INTERNUC. AXIS,3X,
6    8HDE, 1/CM,7X,10HBETA, 1/CM,7X,12HDEZERO, 1/CM,5X,
7    12HPOSITION, CM//
8    1X,11HUPPER STATE,2X,F7.2,17X,I2, 18X,E14.7,1X,E14.7,3X,
9    E14.7,3X,E14.7//
1    1X,11HLOWER STATE,2X,F7.2,17X,I2, 18X,E14.7,1X,E14.7,3X,
2    E14.7,3X,E14.7////)
607  FORMAT(12X,10HELECTRONIC,4X,10HELECTRONIC/
1    12X,10HDEGENERACY,4X,11HTERM ENERGY,4X,2HWE,13X,4HWEZE,11X,
2    4HWEYE,11X,4HWEZE,11X,2HBE,13X,7HALPHA E//)

```

C FORMATS FOR ERROR STATEMENTS.

```

700  FORMAT(/10X,3HTHE,1X,A6,12H BAND SYSTEM,20H IS NOT ON THE TAPE.)
701  FORMAT(/1X,112HERROR - ELECTRONIC TERM ENERGY OF THE UPPER STATE
1    1IS LESS THAN OR EQUAL TO THE TERM ENERGY OF THE LOWER STATE. )

```

C FORMATS FOR TAPE READ STATEMENTS.

```

900  FORMAT(A6,2I6)
901  FORMAT(5E14.7)
902  FORMAT(8E14.7)

```

END

```

$ORIGIN      ALPHA
$IBFTC HF075D

```

SUBROUTINE VU VL (SKIPVV)

C SUBROUTINE VU VL COMPUTES AND READS VIBRATIONAL BAND CONSTANTS
C AND DETERMINES THE MAXIMUM ROTATIONAL QUANTUM NUMBER AND THE INTENSITY
C FACTOR.

```

COMMON/CPL0T/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/ILAM( 9000),ELAM( 9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
1    ALPHA,BEL,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL,TERML
COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,MU,ALTNAT,
1    WEL,WEXEL,WEYEL,WEZEL,BVL,DVL,      KUSPIN
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
COMMON/CTRAN/PARTCC,NUBARO,G,A0E,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

```

```

REAL MU,KMAX2,KMAX1,NUBARO,LOWER,ILAM,NAME
DIMENSION QVV(20)
INTEGER FLAG
DATA UPPER/6HUPPER /, LOWER/6HLOWER /

```

```

SKIPVV= 0.0
A0E=2.5415785E-18
C=2.9979E+10
PI=3.1415927

```

```

VU=READ1
VL=READ2
KMIN=READ3
KMAX=READ4

```

C TEST VIBRATIONAL QUANTUM NUMBERS TO ENSURE THAT FICTITIOUS PEAK IN
C VIBRATIONAL TERM ENERGY HAS NOT BEEN EXCEEDED.

C UPPER STATE.

```

FLAG = 0
WE = WEU
WEXE = WEXEU
WEYE = WEYEU
WEZE = WEZEU
MV = VU + 1.1
GO TO 10

```

```

C LOWER STATE.

5  WE = WEL
   WEXE = WEXEL
   WEYE = WEYEL
   WEZE = WEZEL
   MV = VL +1.1

10 EV1 =0.0
   FLAG = FLAG +1
   DO 20 M=1,MV
     V = M-1
     EV2 =WE*(V+.5) -WEXE*(V+.5)**2+WEYE*(V+.5)**3 +WEZE*(V+.5)**4
     IF(EV2 .LE. EV1) GO TO 230
20  EV1 = EV2

   IF(FLAG.EQ.1) GO TO 5

C COMPUTE ROTATIONAL CONSTANTS FOR THIS BAND.

30  BVU=BEU-ALPHAU*(VU+0.5)
     BVL=BEL-ALPHA*(VL+0.5)
     DVU=DEU+BETAU*(VU+0.5)
     DVL=DEL+BETAL*(VL+0.5)

C READ VIBRATIONAL BAND CONSTANTS.

   READ(5,500) SUMRE2,WIDTHG,WIDTHL,NUBARO,FRANCK,RANGE

C IF A FRANCK-CONDON FACTOR WAS READ, CONTINUE WITH
C THE SOLUTION. IF ONE WAS NOT READ AND THE MOLECULAR AND SPECTROSCOPIC
C CONSTANTS WERE NOT READ FROM TAPE, THEN THE SOLUTION CANNOT PROCEED.

   IF (FRANCK .GT. 0.0) GO TO 40
   IF (NFILE .EQ. 0) GO TO 240

C READ FRANCK-CONDON FACTORS FROM TAPE USING THE WEZE ARRAY FOR
C TEMPORARY STORAGE.

   CALL SKIP(-0,9)
   READ(9,900) NAME,INDEX,NFILE
   N1=VU+1.1
   N2=VL+1.1
   READ(9,901) ((QVV(M2),M2=1,20),M1=1,N1)
   FRANCK=QVV(N2)

C RANGE IS THE DISTANCE FROM THE LINE CENTER, IN LINE WIDTHS, BEYOND
C WHICH THE SPONTANEOUS LINE EMISSION IS CONSIDERED ZERO.

40  IF(RANGE .NE. 0.0) GO TO 45
     RANGE=5.0
     IF (WIDTHL .EQ. 0.0) RANGE=3.0

C FIND THE VOIGT LINE WIDTH AT HALF-HEIGHT. IF LINE WIDTHS WERE NOT INPUT
C IMPOSE A GAUSSIAN PROFILE WITH A WIDTH TEN TIMES DELLAM.

45  WIDTHV=WIDTHL/2.0+SQRT(WIDTHL**2/4.0+WIDTHG**2)
     IF (WIDTHV .NE. 0.0) GO TO 50
     WIDTHV=10.0*DELLAM
     WIDTHG=WIDTHV
     WRITE(6,701)

C FIND KMAX, THE MAXIMUM ROTATIONAL QUANTUM NUMBER POSSIBLE FOR THE
C SPECIFIED VIBRATIONAL LEVELS. KMAX VALUES ARE FOUND FOR BOTH THE
C UPPER AND LOWER STATES. HOWEVER, VALUE OF THE KMAX USED BY THE PROGRAM
C IS THE MINIMUM OF THESE AND THE INPUT VALUE IF IT IS NOT ZERO. IF THE
C DISSOCIATION ENERGY IS NOT INPUT, KMAX CANNOT BE DETERMINED AND IS SET TO
C THE INPUT VALUE OR 150 IF THE INPUT VALUE IS ZERO.
C SEE HERZBERG, PAGE 426, FOR A DISCUSSION OF DISSOCIATION DUE TO ROTATION.

C SET UP CONSTANTS TO FIND KMAX FOR LOWER STATE.

50  IF (DZEROL .EQ. 0.0) GO TO 60

     DEQUIL=DZEROL +WEL/2.0 -WEXEL/4.0 +WEYEL/8.0 +WEZEL/16.0
     EVIB=WEL*(VL+0.5) -WEXEL*(VL+0.5)**2 +WEYEL*(VL+0.5)**3
     1 +WEZEL*(VL+0.5)**4
     C1=1.2177E7*WEL*SQRT(MU/DEQUIL)
     REQUIL=REL
     DV=DVL
     BV=BVL
     GO TO 70

C SET UP CONSTANTS TO FIND KMAX FOR UPPER STATE.

60  IF (DZEROU .EQ. 0.0) GO TO 170

     DEQUIL=DZEROU +WEU/2.0 -WEXEU/4.0 +WEYEU/8.0 +WEZEU/16.0
     EVIB=WEU*(VU+0.5) -WEXEU*(VU+0.5)**2 +WEYEU*(VU+0.5)**3
     1 +WEZEU*(VU+0.5)**4
     C1=1.2177E7*WEU*SQRT(MU/DEQUIL)
     REQUIL=REU
     DV=DVU
     BV=BVU

C IF VIBRATIONAL ENERGY IS GREATER THAN OR EQUAL TO THE DISSOCIATION
C ENERGY, THIS BAND CANNOT EXIST.

70  IF (EVIB .GE. DEQUIL) GO TO 220

```

```

C SET THE INITIAL VALUES NEEDED TO START THE ITERATION.
C KMAX1= PRIOR VALUE OF KMAX
C KMAX2= PRESENT VALUE OF KMAX
C KMAX3= INTEGER VALUE OF NEXT KMAX
C K= INTEGER VALUE OF KMAX2
C E1 AND E2= PRIOR AND PRESENT SUMS OF VIBRATIONAL PLUS ROTATIONAL ENERGY.
C U1 AND U2= PRIOR AND PRESENT VALUES OF EFFECTIVE POTENTIAL ENERGY AT THE
C LOCAL MAXIMUM.
C FLAG=1 INDICATES THIS IS THE FIRST ITERATION.

      C3=1.686E-15/MU
      E1=EVIB
      U1=DEQUIL
      KMAX1=0.0
      K= 50
      KMAX2=K
      FLAG= 1

C FIND R, THE INTERNUCLEAR DISTANCE AT THE LOCAL MAXIMUM OF THE
C EFFECTIVE POTENTIAL WELL FOR KMAX2. A MORSE CURVE IS ASSUMED
C FOR THE POTENTIAL WELL WITHOUT ROTATION.

80   R=REQUIL
      FR2=0.0
      FK=C3*1.0E+24*KMAX2*(KMAX2+1.0)/(C1*DEQUIL)

90   FR1=FR2
      R=R+0.1E-8
      IF (R .GT. 1.0E-7) GO TO 120

      C2=EXP(-C1*(R-REQUIL))
      FR2=(R *1.0E+8)**3*C2*(1.0-C2)
      IF (FR2 .GT. FR1) GO TO 90
      IF (FR2 .GT. FK) GO TO 90
      IF (FR1 .EQ. FR2) GO TO 100
      IF (FR1 .GT. FK) GO TO 110

C A LOCAL MAXIMUM DOES NOT EXIST AT K.
C SET R TO PRIOR VALUE AND CONTINUE ITERATION.

      R= R-0.1E-8
      GO TO 120

C THE LOCAL MAXIMUM AT K IS, IN FACT, A CRITICAL POINT.
C SET R TO CRITICAL POINT AND CONTINUE ITERATION.

100  R=R- 0.05E-8
      GO TO 120

C INTERPOLATE TO GET VALUE OF R AT LOCAL MAXIMUM.

110  R=R- 0.1E-8*(FK-FR2)/(FR1-FR2)

C FIND THE NEXT VALUE OF KMAX (I.E., KMAX3). DURING THE FIRST ITERATION
C STEP KMAX2 BY 20 UNTIL U2 IS LESS THAN OR EQUAL TO E2 AND THEN
C INTERPOLATE TO U=E TO GET KMAX3. IN ALL OTHER ITERATIONS, JUST
C EXTRAPOLATE TO U=E TO GET KMAX3.

120  E2=EVIB +BV*KMAX2*(KMAX2+1.0) -DV*KMAX2**2*(KMAX2+1.0)**2
      U2=DEQUIL*(1.0-EXP(-C1*(R-REQUIL)))**2 +C3*KMAX2*(KMAX2+1.0)/R**2

      IF (FLAG .NE. 1) GO TO 140
      IF (U2 .LE. E2) GO TO 130
      KMAX1= KMAX2
      KMAX2= KMAX2+ 20.0
      K= KMAX2+ 0.1

      IF (KMAX2 .GE. 500.0) GO TO 150

      E1= E2
      U1= U2
      GO TO 120

130  FLAG= 2
140  KMAX3=KMAX2 +(U2-E2)*(KMAX2-KMAX1)/((U1-E1)-(U2-E2))

C IF KMAX3 IS LESS THAN OR EQUAL TO ZERO, THIS VIBRATIONAL LEVEL
C CANNOT EXIST.

      IF (KMAX3 .LE. 0) GO TO 260

C WHEN KMAX3 EQUALS K, THE ITERATION IS COMPLETE.

      IF (KMAX3 .EQ. K) GO TO 160
      K=KMAX3
      KMAX1=KMAX2
      KMAX2=KMAX3
      E1=E2
      U1=U2
      GO TO 80

150  KMAX3= KMAX2+ 0.1

C THE ITERATION IS COMPLETE, SET KMAX.

160  IF (KMAX .EQ. 0) KMAX=KMAX3
      IF (KMAX3 .LT. KMAX) KMAX=KMAX3
      IF (BV .EQ. BVL) GO TO 60
      IF (KMAX .EQ. 0) KMAX=150

```

```

C SET UP CONSTANTS FOR INTENSITY EQUATION IN ROTATIONAL STRUCTURE
C SUBROUTINE AND COMPUTE NUBARO, THE BAND ORIGIN, IF NOT SPECIFIED.

      CINT1=TERMU/TELECT + (WEU*(VU+0.5)-WEXEU*(VU+0.5)**2+WYEU*
1      (VU+0.5)**3+WEZEU*(VU+0.5)**4)/TVIB

      CINT2=(16.0E-7*C*PARTCC*FRANCK*SUMRE2*PI**3)/(3.0*Q)

      IF (NUBARO .EQ. 0.0) NUBARO=TERMU -TERML +WEU*(VU+0.5) -WEXEU*
1      (VU+0.5)**2 +WYEU*(VU+0.5)**3
2      +WEZEU*(VU+0.5)**4 -WEL*(VL+0.5)
3      +WEXEL*(VL+0.5)**2 -WYEL*(VL+0.5)**3
4      -WEZEL*(VL+0.5)**4
      ORIGIN=1.0E+8/NUBARO

C FIND THE INTENSITY FACTOR, IF NECESSARY.

      IFACR= 0.62486*CINT1
      IF (IFACR .LT. 30) GO TO 210
      CINT4=IFACR
      IF (CINT4 .LT. CINT3) GO TO 210

      FACTR(1)=OUTPUT(12)
      M=IFACR/1000
      DO 180 M1=2,5
        FACTR(M1)=OUTPUT(M+1)
        IFACR=IFACR-M*10**(5-M1)
180      M=IFACR/10**(4-M1)

C IF THIS IS NOT THE FIRST INTENSITY FACTOR, ADJUST THE ELAM ARRAY.

      IF (CINT3 .EQ. 0.0) GO TO 200
      CINT5= CINT4-CINT3
      DO 190 M=1,NARRAY
190      ELAM(M)=ELAM(M)*EXP(2.30259*CINT5)

      SYSTEM= SYSTEM*EXP(2.30259*CINT5)
      TOTAL= TOTAL*EXP(2.30259*CINT5)
200      CINT3= CINT4

C WRITE THE VIBRATIONAL BAND INFORMATION.

210      M1=VU+ 0.1
      M2=VL+ 0.1
      IRANGE= RANGE+ 0.1
      IF (KMIN .LT. 2) KMIN= 2

      WRITE(6,600)M1,M2,FRANCK,SUMRE2,WIDTHG,WIDTHL,WIDTHV,IRANGE,
1      ORIGIN,KMIN,KMAX
      IF (CINT2 .LE. 0.0) GO TO 250
      RETURN

C THIS VIBRATIONAL LEVEL CANNOT EXIST. WRITE THE APPROPRIATE MESSAGE
C AND OMIT THIS BAND.

220      M1=VU+ 0.1
      M2=VL+ 0.1
      DUMMY=UPPER
      IF (BV .EQ. BVL) DUMMY=LOWER
      WRITE(6,702) M1,M2,DUMMY
      SKIPVV= 1.0
      RETURN

230      M1=VU+ 0.1
      M2=VL+ 0.1
      DUMMY=UPPER
      IF (WE .EQ. WEL) DUMMY=LOWER
      WRITE(6,705) M1,M2,DUMMY
      READ(5,500) SUMRE2,WIDTHG,WIDTHL,NUBARO,FRANCK,RANGE
      SKIPVV= 1.0
      RETURN

C THERE IS AN ERROR IN THE FRANCK-CONDON FACTOR. WRITE AN ERROR MESSAGE
C AND OMIT THIS BAND.

240      M1= VU+ 0.1
      M2= VL+ 0.1
      WRITE(6,703) M1,M2
      SKIPVV= 1.0
      RETURN

C THE BAND INTENSITY IS ZERO DUE TO A POSSIBLE ERROR IN PARTCC, FRANCK, SUMRE2,
C OR Q. WRITE THE APPROPRIATE MESSAGE AND OMIT THIS BAND.

250      WRITE(6,700)
      SKIPVV= 1.0
      RETURN

C THE MAX POSSIBLE ROTATIONAL QUANTUM NUMBER IS LESS THAN OR EQUAL
C TO ZERO. WRITE THE APPROPRIATE MESSAGE AND OMIT THIS BAND.

260      M1= VU+ 0.1
      M2= VL+ 0.1
      WRITE(6,704) M1,M2
      SKIPVV= 1.0
      RETURN

C FORMAT FOR READ STATEMENT.

```

```

500  FORMAT(6E10.0)

C  FORMAT FOR WRITE STATEMENT.

600  FORMAT(/1X,I2,4X,I2,6X,1PE10.4,3X,E10.4,9X,3(OPF7.4,1X),3X,I4,
1      7X,F9.3,5X,I4,5X,I4//)

C  FORMATS FOR ERROR STATEMENTS.

700  FORMAT(/2X,130HINTENSITY FOR THIS BAND IS LESS THAN OR EQUAL TO ZE
1RO DUE TO THE INPUT DATA VALUES. THEREFORE IT WAS OMITTED FROM THE
2  COMPUTATION.)
701  FORMAT(/8X,117HLINE WIDTHS WERE NOT INPUT FOR NEXT BAND. PROGRAM I
2) IMPOSED A GAUSSIAN PROFILE WITH WIDTH AT HALF-HEIGHT = 10*INTERVAL.
702  FORMAT(/6X,4HTHE ,I2,3H , ,I2,84H TRANSITION WAS OMITTED FROM THE
1  CALCULATION BECAUSE THE VIBRATIONAL ENERGY FOR THE ,A6,14HSTATE E
2XCEEDED/
3      6X,23HITS DISSOCIATION ENERGY)
703  FORMAT(/10X,41HNO FRANCK-CONDON FACTOR WAS INPUT FOR THE,I2,
1      3H , ,I2, 6H BAND.)
704  FORMAT(/6X,4HTHE ,I2,3H , ,I2,95H TRANSITION WAS OMITTED BECAUSE T
1HE MAX POSSIBLE ROT QUANTUM NUMBER IS LESS THAN OR EQUAL TO 0.//)
705  FORMAT(/6X,4HTHE ,I2,3H , ,I2,92H TRANSITION WAS OMITTED FROM THE
1  CALCULATION BECAUSE THE VIBRATIONAL QUANTUM NUMBER FOR THE ,A6,
25HSTATE/6X,65HEXCEEDS THE FICTITIOUS PEAK ON THE VIBRATIONAL TEM
3ENERGY CURVE.)

C  FORMATS FOR THE TAPE STATEMENTS.

900  FORMAT(A6,2I6)
901  FORMAT(5E14.7)

END
*****

$ORIGIN      ALPHA
$IBFTC HF075E

SUBROUTINE ZERO

C  SUBROUTINE ZERO COMPUTES PARALLEL TRANSITIONS FOR DIATOMIC MOLECULES.

COMMON/CPL0T/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/ILAM( 9000),ELAM( 9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
1      ALPHAL,BEL,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL,TERML
COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,MU,ALTNAT,
1      WEL,WEXEL,WEYEL,WEZEL,BVL,DVL,      NUSPIN
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
COMMON/CTRAN/PARTCC,NUBARO,Q,AOE,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

REAL ILAM,KU,KL,LAMCL,LAMBDA,LAMMAX,LAMMIN,NUBAR,NUBARO,NUSPIN

C  FIND THE NUMBER OF ENTRIES IN THE INTENSITY ARRAY, FROM THE LINE CLNTER,
C  AT WHICH EACH LINE IS ASSUMED TO HAVE A CONTRIBUTION.

NSPRD=1.1+RANGE*WIDTHV/DELLAM

C  SET CONSTANTS WHICH DETERMINE THE LINE SHAPE.

CSPRD2=WIDTHL/WIDTHV
CSPRD3=(1.065+0.447*CSPRD2+0.058*CSPRD2**2)*WIDTHV*1.0E-4
CSPRD1=(1.0-CSPRD2)/CSPRD3
CSPRD2=CSPRD2/CSPRD3

C  SET CONSTANTS WHICH DETERMINE THE WAVELENGTH OF THE LINE CENTER FOR
C  TRIPLETS.  SEE HERZBERG, PAGE 235.

YU=CAPAU/BVU
YL=CAPAL/BVL
DIVISR=2.0
IF (CAPLU.EQ. 0.0) DIVISR=1.0

C  SET CONSTANTS FOR THE P BRANCH AND INITIALIZE THE RUNNING SUMS.

CSTR=1.0
KU=KMIN
KL=KU+1.0
BAND=0.0

10  BRANCH=0.0

C  COMPUTE AND DISTRIBUTE THE INTEGRATED INTENSITY DUE TO SPONTANEOUS
C  EMISSION OF ALL SPECIFIED ROTATIONAL LINES.

DO 60  M=KMIN,KMAX
Z2U=0.0
Z2L=0.0

C  FOR A DESCRIPTION OF THESE EQUATIONS, SEE HERZBERG, PAGE 235.

IF (DEGENU/DIVISR.NE. 3.0) GO TO 20
Z1U=CAPLU**2*YU*(YU-4.0)+(4.0/3.0)+4.0*KU*(KU+1.0)
Z1L=CAPLL**2*YL*(YL-4.0)+(4.0/3.0)+4.0*KL*(KL+1.0)
Z2U=(CAPLU**2*YU*(YU-1.0)-(4.0/9.0)-2.0*KU*(KU+1.0))/(3.0*Z1U)
Z2L=(CAPLL**2*YL*(YL-1.0)-(4.0/9.0)-2.0*KL*(KL+1.0))/(3.0*Z1L)

```

```

C COMPUTE THE WAVELENGTH OF THE LINE CENTER IN ANGSTROMS.
20  NUBAR=NUBARO +BVU*(KU*(KU+1.0)+4.0*Z2U) -BVL*(KL*(KL+1.0)+4.0*
1    Z2L) -DVU*(KU+0.5)**4 +DVL*(KL+0.5)**4
    LAMCL=1.0E+8/NUBAR
C IF THE LINE WAVELENGTH FALLS OUTSIDE THE SPECTRAL RANGE OF
C INTEREST, OMIT IT AND PROCEED TO THE NEXT LINE.
    IF(LAMCL.LT.LAMMIN-RANGE*WIDTHV) GO TO 50
    IF(LAMCL.GT.LAMMAX+RANGE*WIDTHV) GO TO 50
C FIND THE STRENGTH FACTOR.
    S=KU+CSTR
C DETERMINE IF LINES ALTERNATE IN INTENSITY.
    FACTOR=1.0
    IF (ALTNAT .EQ. 0.0) GO TO 30
C EVALUATE THE ALTERNATION FACTOR FOR HOMONUCLEAR MOLECULES. THE
C EXPONENT IN THE ALTERNATING FUNCTION IS FOUND SEPARATELY TO ENSURE
C THAT IT IS AN INTEGER BEFORE RAISING (-1.0) TO A POWER.
    KEXP= KL + ALTNAT + 0.1
    FACTOR=1.0 +(-1.0)**KEXP/(2.0*NUSPIN+1.0)
C FIND THE INTEGRATED LINE INTENSITY DUE TO SPONTANEOUS EMISSION.
30  E=FACTOR*S*(NUBAR**2*A0E)**2*CINT2*EXP(-1.43879*(CINT1
1    +(BVU*KU*(KU+1.0))/TROT)+2.30259*CINT3)
C SET CONSTANTS USED TO DISTRIBUTE THE ROTATIONAL LINE.
    NCENTR=1.5+(LAMCL-LAMMIN)/DELLAM
    NSTART=NCENTR-NSPRE
    IF (NSTART .LT. 1) NSTART=1
    NEND=NCENTR +NSPRE
    IF (NEND .GT. NARRAY) NEND=NARRAY
C DISTRIBUTE THE ROTATIONAL LINE.
    DO 40 M1=NSTART,NEND
    COUNT=M1
    LAMBDA=LAMMIN+(COUNT-1.0)*DELLAM
    CSPRD3=ABS((LAMBDA-LAMCL)/WIDTHV)
40  ELAM(M1)=ELAM(M1) +E*(CSPRD1*EXP(-2.772*CSPRD3**2)
1    +CSPRD2/(1.0+4.0*CSPRD3**2) +0.016* CSPRD2*(1.0-
2    WIDTHL/WIDTHV)*(EXP(-0.4*CSPRD3**2.25) -10.0/
3    (10.0+CSPRD3**2.25)))
    BRANCH= BRANCH + E
50  KU=KU+1.0
60  KL=KL+1.0
C HAVE BOTH BRANCHES BEEN COMPLETED.
    IF (KL .EQ. KU-1.0) GO TO 70
C WRITE P BRANCH DATA.
    WRITE(6,600) BRANCH,(FACTRI(M),M=1,5)
    BAND=BRANCH
    SYSTEM=SYSTEM+BRANCH
C SET CONSTANTS FOR THE R BRANCH.
    CSTR=0.0
    KU=KMIN
    KL=KU-1.0
    GO TO 10
C WRITE R BRANCH DATA.
70  WRITE(6,601) BRANCH,(FACTRI(M),M=1,5)
    BAND=BAND+BRANCH
    SYSTEM=SYSTEM+BRANCH
C COMPUTE APPROXIMATE BAND INTENSITY. SEE BATES, PAGE 57.
    QR=TROT/(1.43879*BVU)
    APPROX=CINT2*QR*(NUBARO**2*A0E)**2*EXP(-1.43879*CINT1+
1    2.30259*CINT3)
C WRITE ADDITIONAL DATA FOR THIS VIBRATIONAL BAND.
    WRITE(6,602) BAND,(FACTRI(M),M=1,5),APPROX,(FACTRI(M),M=1,5)
    RETURN
C FORMATS FOR WRITE STATEMENTS.
600  FORMAT(107X,8HP BRANCH,1X,1PE10.4,5A1)
601  FORMAT(107X,8HP BRANCH,1X,1PE10.4,5A1)
602  FORMAT(/ 105X,10HBAND TOTAL,1X,1PE10.4,5A1/
1    93X,22HAPPROXIMATE BAND TOTAL,1X,E10.4,5A1//)
END
*****

```

SORIGIN ALPHA
SIBFTC HF075F

SUBROUTINE ONE

C SUBROUTINE ONE COMPUTES PERPENDICULAR TRANSITIONS FOR DIATOMIC
C MOLECULES.

```
COMMON/CPLT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/ILAM( 9000),ELAM( 9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
1  ALPHAL,BEL,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL,TERML
COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,MU,ALTNAT,
1  WEL,WEXEL,WEYEL,WEZEL,BVL,DVL, NUSPIN
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
COMMON/CTRAN/PARTCC,NUBAR0,Q,AOE,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

REAL ILAM,KU,KL,LAMCL,LAMBDA,LAMMAX,LAMMIN,NUBAR,NUBAR0,NUSPIN
INTEGER SWITCH
```

C FIND THE NUMBER OF ENTRIES IN THE INTENSITY ARRAY, FROM THE LINE CENTER,
C AT WHICH EACH LINE IS ASSUMED TO HAVE A CONTRIBUTION.

```
NSPRED=1.1+RANGE*WIDTHV/DELLAM
```

C SET CONSTANTS WHICH DETERMINE THE LINE SHAPE.

```
CSPRD2=WIDTHL/WIDTHV
CSPRD3=(1.065+0.447*CSPRD2+0.058*CSPRD2**2)*WIDTHV*1.0E-4
CSPRD1=(1.0-CSPRD2)/CSPRD3
CSPRD2=CSPRD2/CSPRD3
```

C SET THE SIGN OF CAPLU, USED IN STRENGTH EQUATIONS, APPROPRIATE TO THE
C SIGN OF DELTA LAMBDA. SEE JOHNSON, PAGE 150.

```
SIGN=1.0
IF (CAPLU .LT. CAPLL) SIGN=-1.0
```

C SET CONSTANTS FOR THE P BRANCH AND INITIALIZE THE RUNNING SUMS.

```
SWITCH= 1
KU=KMIN
KL=KU+1.0
BAND = 0.0
10  BRANCH=0.0
```

C COMPUTE AND DISTRIBUTE THE INTEGRATED INTENSITY DUE TO SPONTANEOUS
C EMISSION OF ALL SPECIFIED ROTATIONAL LINES.

```
DO 90 M=KMIN,KMAX
```

C COMPUTE THE WAVELENGTH OF THE LINE CENTER IN ANGSTROMS.

```
NUBAR=NUBAR0 +BVU*KU*(KU+1.0) -BVL*KL*(KL+1.0) -DVU*KU**2*
1  (KU+1.0)**2 +DVL*KL**2*(KL+1.0)**2
LAMCL=1.0E+8/NUBAR
```

C IF THE LINE WAVELENGTH FALLS OUTSIDE THE SPECTRAL RANGE OF
C INTEREST, OMIT IT AND PROCEED TO THE NEXT LINE.

```
IF(LAMCL.LT.LAMMIN-RANGE*WIDTHV) GO TO 80
IF(LAMCL.GT.LAMMAX+RANGE*WIDTHV) GO TO 80
```

C FIND THE STRENGTH FACTOR.

```
GO TO (20,30,40), SWITCH
```

C P BRANCH STRENGTH FACTOR

```
20  S=(KU+1.0-SIGN*CAPLU)*(KU+2.0-SIGN*CAPLU)/(2.0*(KU+1.0))
GO TO 50
```

C Q BRANCH STRENGTH FACTOR.

```
30  S=(KU+SIGN*CAPLU)*(2.0*KU+1.0)*(KU+1.0-SIGN*CAPLU)/
1  (2.0*KU*(KU+1.0))
GO TO 50
```

C R BRANCH STRENGTH FACTOR.

```
40  S=(KU+SIGN*CAPLU)*(KU-1.0+SIGN*CAPLU)/(2.0*KU)
```

C DETERMINE IF LINES ALTERNATE IN INTENSITY.

```
50  FACTOR=1.0
IF (ALTNAT .EQ. 0.0) GO TO 60
```

C EVALUATE THE ALTERNATION FACTOR FOR HOMONUCLEAR MOLECULES. THE
C EXPONENT IN THE ALTERNATING FUNCTION IS FOUND SEPARATELY TO ENSURE
C THAT IT IS AN INTEGER BEFORE RAISING (-1.0) TO A POWER.

```
KEXP= KL + ALTNAT + 0.1
FACTOR=1.0 +(-1.0)**KEXP/(2.0*NUSPIN+1.0)
```

```

C FIND THE INTEGRATED LINE INTENSITY DUE TO SPONTANEOUS EMISSION.
60 E=FACTOR*S*(NUBAR**2*AOE)**2*CINT2*EXP(-1.43879*(CINT1
1 +(BVU*KU*(KU+1.0))/TROT)+2.30259*CINT3)
C SET CONSTANTS USED TO DISTRIBUTE THE ROTATIONAL LINE.
NCENTR=1.5+(LAMCL-LAMMIN)/DELLAM
NSTART=NCENTR-NSPRED
IF (NSTART .LT. 1) NSTART=1
NEND=NCENTR +NSPRED
IF (NEND .GT. NARRAY) NEND=NARRAY
C DISTRIBUTE THE ROTATIONAL LINE.
DO 70 M1=NSTART,NEND
COUNT=M1
LAMBDA=LAMMIN+(COUNT-1.0)*DELLAM
CSPRD3=ABS((LAMBDA-LAMCL)/WIDTHV)
70 ELAM(M1)=ELAM(M1) +E*(CSPRD1*EXP(-2.772*CSPRD3**2)
1 +CSPRD2/(1.0+4.0*CSPRD3**2) +0.016* CSPRD2*(1.0-
2 WIDTHL/WIDTHV)*(EXP(-0.4*CSPRD3**2.25) -10.0/
3 (10.0+CSPRD3**2.25)))
BRANCH= BRANCH + E
80 KU=KU+1.0
90 KL=KL+1.0
BAND=BAND+BRANCH
SYSTEM=SYSTEM+BRANCH
C HAVE ALL THREE BRANCHES BEEN COMPLETED.
GO TO (100,110,120),SWITCH
C OUTPUT P BRANCH INTEGRATED INTENSITY.
100 WRITE(6,600) BRANCH,(FACTRI(M),M=1,5)
C SET CONSTANTS FOR Q BRANCH.
SWITCH= 2
KU=KMIN
KL=KU
GO TO 10
C OUTPUT Q BRANCH INTEGRATED INTENSITY.
110 WRITE(6,601) BRANCH,(FACTRI(M),M=1,5)
C SET CONSTANTS FOR R BRANCH.
SWITCH= 3
KU=KMIN
KL=KU-1.0
GO TO 10
C OUTPUT R BRANCH INTEGRATED INTENSITY.
120 WRITE(6,602) BRANCH,(FACTRI(M),M=1,5)
C COMPUTE APPROXIMATE BAND INTENSITY. SEE BATES, PAGE 57.
QR=TROT/(1.43879*BVU)
APPROX=CINT2*QR*(NUBARO**2*AOE)**2*EXP(-1.43879*CINT1+
1 2.30259*CINT3)
WRITE(6,603) BAND,(FACTRI(M),M=1,5),APPROX,(FACTRI(M),M=1,5)
RETURN
C FORMATS FOR WRITE STATEMENTS.
600 FORMAT(107X,8HP BRANCH,1X,1PE10.4,5A1)
601 FORMAT(107X,8HQ BRANCH,1X,1PE10.4,5A1)
602 FORMAT(107X,8HR BRANCH,1X,1PE10.4,5A1)
603 FORMAT(/ 105X,10HBAND TOTAL,1X,1PE10.4,5A1/
1 93X,22HAPPROXIMATE BAND TOTAL,1X,E10.4,5A1//)
END
*****
$ORIGIN ALPHA
$IBFTC HF075G
SUBROUTINE S2 PI2
C SUBROUTINE S2 PI2 COMPUTES DOUBLET SIGMA TO DOUBLET PI TRANSITIONS (OR
C VICE VERSA) FOR DIATOMIC MOLECULES.
COMMON/CPL0T/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/ILAM( 9000),ELAM( 9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
1 ALPHAL,BEL,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL,TERML
COMMON/CBAND2/WEU,WEXEU,WYEU,WZEU,BVU,DVU,DEGENU,MU,ALTNAT,
1 WEL,WEXEL,WYEL,WZEL,BVL,DVL, NUSPIN
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
COMMON/CTRAN/PARTCC,NUBARO,Q,AOE,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

```

```

      DIMENSION NAME(16,2)
      REAL ILAM,J,JL,JU,K,LAMCL,LAMBDA,LAMMAX,LAMMIN,NUBAR,NUBARO,
      1 NUSPIN
      INTEGER SWITCH
      LOGICAL FROMPI,DBLBRN
      DATA((NAME(M1,M2),M2=1,2),M1=1,16)/

C      PI TO SIGMA TRANS.          SIGMA TO PI TRANS.

      1 6H ,6H P2 ,          6H ,6H R2 ,
      2 6H ,6H R1 ,          6H ,6H P1 ,
      3 6H ,6H SR21 ,        6H ,6H SR21 ,
      4 6H ,6H OP12 ,        6H ,6H OP12 ,
      5 6HQ2 AND,6H QP21 ,    6HQ2 AND,6H QR12 ,
      6 6HQ1 AND,6H QR12 ,    6HQ1 AND,6H QP21 ,
      7 6HR2 AND,6H RQ21 ,    6HP2 AND,6H PQ12 ,
      8 6HP1 AND,6H PQ12 ,    6HR1 AND,6H RQ21 /

C DBLBRN IS TRUE WHEN COMPUTING TWO BRANCHES WHOSE LINES ARE ASSUMED TO
C HAVE THE SAME WAVELENGTHS.

      DBLBRN=.FALSE.

C ADJUST FACTOR USED IN INTENSITY EQUATION TO ACCOUNT FOR SPIN SPLITTING.

      CINT2=CINT2/2.0

C SET CONSTANTS APPROPRIATE TO THE ELECTRONIC TRANSITION. FROMPI IS TRUE
C IF THE UPPER STATE IS DOUBLET P1.

      FROMPI=.FALSE.
      IF (CAPLU.GT.CAPLL) FROMPI=.TRUE.

C SET COUPLING CONSTANT.

      YU=CAPAU/BVU
      YL=CAPAL/BVL
      Y=YL
      IF (FROMPI) Y=YU

C SET SWITCH, THE BRANCH IDENTIFIER, AND IPRINT, THE INDEX ON NAME WHICH
C IDENTIFIES THE BRANCH OUTPUT.

      SWITCH= 0
      IPRINT=0
      IF (FROMPI) IPRINT=-1

C FIND THE NUMBER OF ENTRIES IN THE INTENSITY ARRAY, FROM THE LINE CENTER,
C AT WHICH EACH LINE IS ASSUMED TO HAVE A CONTRIBUTION.

      NSPRD=1.1+RANGE*WIDTHV/DELLAM

C SET CONSTANTS WHICH DETERMINE THE LINE SHAPE.

      CSPRD2=WIDTHL/WIDTHV
      CSPRD3=(1.065+0.447*CSPRD2+0.058*CSPRD2**2)*WIDTHV*1.0E-4
      CSPRD1=(1.0-CSPRD2)/CSPRD3
      CSPRD2=CSPRD2/CSPRD3

C SET CONSTANTS FOR THE P2 BRANCH (PI TO SIGMA TRANSITION) OR
C R2 BRANCH (SIGMA TO PI TRANSITION).

      BAND=0.0
      K=KMIN
      JU=K-0.5
      JL=JU-1.0
      IF (FROMPI) JL=JU+1.0

C SET CONSTANTS FOR THE WAVELENGTH EQUATION.

      SIGNU1=1.0
      SIGNU2=1.0

C SET CONSTANTS FOR THE STRENGTH EQUATION.

      SIGNS1=1.0
      SIGNS2=-1.0

      CONST1=1.0
      CONST2=1.0
      GO TO 80

10 WRITE(6,600) (NAME(IPRINT,M1),M1=1,2),BRANCH,(FACTRI(M),M=1,5)

C SET CONSTANTS FOR THE R1 BRANCH (PI TO SIGMA TRANSITION) OR
C P1 BRANCH (SIGMA TO PI TRANSITION).

      JU=K+0.5
      JL=JU+1.0
      IF (FROMPI) JL=JU-1.0

C SET CONSTANTS FOR THE WAVELENGTH EQUATION.

      SIGNU1=-1.0
      SIGNU2=-1.0

C SET CONSTANTS FOR THE STRENGTH EQUATION.

```

```

SIGN1=1.0
SIGN2=-1.0

CONST1=1.0
CONST2=0.0
GO TO 80

20  WRITE(6,600) (NAME(IPRINT,M1),M1=1,2),BRANCH,(FACTRI(M),M=1,5)
C  SET CONSTANTS FOR THE SR21 BRANCH (EITHER TRANSITION).

JU=K-0.5
JL=JU-1.0

C  SET CONSTANTS FOR THE WAVELENGTH EQUATION.

SIGNU1=1.0
SIGNU2=-1.0

C  SET CONSTANTS FOR THE STRENGTH EQUATION.

SIGN1=-1.0
SIGN2=-1.0

CONST1=1.0
CONST2=1.0
IF (FROMPI) CONST2=0.0
GO TO 80

30  WRITE(6,600) (NAME(IPRINT,M1),M1=1,2),BRANCH,(FACTRI(M),M=1,5)
C  SET CONSTANTS FOR THE OP12 BRANCH (EITHER TRANSITION).

JU=K+0.5
JL=JU+1.0

C  SET CONSTANTS FOR THE WAVELENGTH EQUATION.

SIGNU1=-1.0
SIGNU2=1.0

C  SET CONSTANTS FOR THE STRENGTH EQUATION.

SIGN1=-1.0
SIGN2=-1.0

CONST1=1.0
CONST2=0.0
IF (FROMPI) CONST2=1.0
GO TO 80

40  WRITE(6,600) (NAME(IPRINT,M1),M1=1,2),BRANCH,(FACTRI(M),M=1,5)
C  SET CONSTANTS FOR THE Q2 AND QP21 BRANCHES (PI TO SIGMA TRANSITION) OR
C  Q2 AND QR12 BRANCHES (SIGMA TO PI TRANSITION).

DBLBRN=.TRUE.
JU=K-0.5
JL=JU

C  SET CONSTANTS FOR THE WAVELENGTH EQUATION.

SIGNU1=1.0
SIGNU2=1.0

C  SET CONSTANTS FOR THE STRENGTH EQUATION.

SIGN1=-1.0
SIGN2=1.0
SIGN3=-1.0

CONST1=-7.0
CONST2=1.0
CONST3=1.0
GO TO 80

50  WRITE(6,602) (NAME(IPRINT,M1),M1=1,2),BRANCH,(FACTRI(M),M=1,5)
C  SET CONSTANTS FOR THE Q1 AND QR12 BRANCHES (PI TO SIGMA TRANSITION) OR
C  Q1 AND QP21 BRANCHES (SIGMA TO PI TRANSITION).

JU=K+0.5
JL=JU

C  SET CONSTANTS FOR THE WAVELENGTH EQUATION.

SIGNU1=-1.0
SIGNU2=-1.0

C  SET CONSTANTS FOR THE STRENGTH EQUATION.

SIGN1=-1.0
SIGN2=1.0
SIGN3=1.0

CONST1=-7.0
CONST2=0.0
CONST3=-7.0
GO TO 80

60  WRITE(6,602) (NAME(IPRINT,M1),M1=1,2),BRANCH,(FACTRI(M),M=1,5)

```

```

C SET CONSTANTS FOR THE R2 AND RQ21 BRANCHES (PI TO SIGMA TRANSITION) OR
C P2 AND PQ12 BRANCHES (SIGMA TO PI TRANSITION).

    JU=K-0.5
    JL=JU+1.0
    IF (FROMPI) JL=JU-1.0

C SET CONSTANTS FOR THE WAVELENGTH EQUATION.

    SIGNU1=1.0
    SIGNU2=1.0

C SET CONSTANTS FOR THE STRENGTH EQUATION.

    SIGNS1=1.0
    SIGNS2= 1.0
    SIGNS3= 1.0

    CONST1=-7.0
    CONST2=0.0
    CONST3=-7.0
    GO TO 80

70 WRITE(6,602) (NAME(IPRINT,M1),M1=1,2),BRANCH,(FACTRI(M),M=1,5)

C SET CONSTANTS FOR THE P1 AND PQ12 BRANCHES (PI TO SIGMA TRANSITION) OR
C R1 AND RQ21 BRANCHES (SIGMA TO PI TRANSITION).

    JU=K+0.5
    JL=JU-1.0
    IF (FROMPI) JL=JU+1.0

C SET CONSTANTS FOR THE WAVELENGTH EQUATION.

    SIGNU1=-1.0
    SIGNU2=-1.0

C SET CONSTANTS FOR THE STRENGTH EQUATION.

    SIGNS1=1.0
    SIGNS2=1.0
    SIGNS3=-1.0

    CONST1=-7.0
    CONST2=1.0
    CONST3=1.0

C COMPUTE AND DISTRIBUTE THE INTEGRATED INTENSITY DUE TO SPONTANEOUS
C EMISSION OF ALL SPECIFIED ROTATIONAL LINES FOR THE APPROPRIATE BRANCH.
C J IS THE ROTATIONAL QUANTUM NUMBER OF THE PI STATE. SEE REFERENCE BY
C EARLS.

80 BRANCH=0.0
   J=JL
   IF (FROMPI) J=JU

   DO 120 M=KMIN,KMAX

C COMPUTE THE WAVELENGTH OF THE LINE CENTER IN ANGSTROMS.

      NUBAR=NUBARO +BVU*((JU+0.5)**2 -CAPLU**2 +SIGNU1/2.0 *SQRT(4.0*
1      (JU+0.5)**2-4.0*YU*CAPLU**2 +(YU*CAPLU)**2))
2      -BVL*((JL+0.5)**2 -CAPLL**2 +SIGNU2/2.0*
3      SQRT(4.0*(JL+0.5)**2 -4.0*YL*CAPLL**2 +(YL*CAPLL)**2))

      LAMCL=1.0E+8/NUBAR

C IF THE LINE WAVELENGTH FALLS OUTSIDE THE SPECTRAL RANGE OF
C INTEREST, OMIT IT AND PROCEED TO THE NEXT LINE.

      IF(LAMCL.LT.LAMMIN-RANGE*WIDTHV) GO TO 110
      IF(LAMCL.GT.LAMMAX+RANGE*WIDTHV) GO TO 110

C FIND STRENGTH FACTOR FOR SINGLE BRANCHES.

      U=1.0/SQRT(Y**2-4.0*Y+(2.0*J+1.0)**2)
      S=((2.0*J+1.0)**2 +SIGNS1*(2.0*J+1.0)*U*(4.0*J**2 +4.0*J +CONST1
1      +SIGNS2*2.0*Y))/(16.0*(J+CONST2))

      IF (.NOT.DBLBRN) GO TO 90

C FIND STRENGTH FACTOR FOR DOUBLE BRANCHES.

      S=S +(2.0*J+1.0)*((4.0*J**2+4.0*J-1.0) -SIGNS1*U*(8.0*J**3+12.0
1      *J**2 -2.0*J +CONST3 +SIGNS3*2.0*Y))/(16.0*J*(J+1.0))

C FIND THE INTEGRATED LINE INTENSITY DUE TO SPONTANEOUS EMISSION.

90 E=S*(NUBAR**2*A0E)**2*CINT2*EXP(-1.43879*(CINT1
1   +(BVU*JU*(JU+1.0))/TROT)+2.30259*CINT3)

C SET CONSTANTS USED TO DISTRIBUTE THE ROTATIONAL LINE.

    NCENTR=1.5+(LAMCL-LAMMIN)/DELLAM
    NSTART=NCENTR-NSPRED
    IF (NSTART .LT. 1) NSTART=1
    NEND=NCENTR +NSPRED
    IF (NEND .GT. NARRAY) NEND=NARRAY

```

C DISTRIBUTE THE ROTATIONAL LINE.

```

      DO 100 M1=NSTART,NEND
      COUNT=M1
      LAMBDA=LAMMIN+(COUNT-1.0)*DELLAM
      CSPRD3=ABS((LAMBDA-LAMCL)/WIDTHV)
100   ELAM(M1)=ELAM(M1) +E*(CSPRD1*EXP(-2.772*CSPRD3**2)
      1      +CSPRD2/(1.0+4.0*CSPRD3**2) +0.016* CSPRD2*(1.0-
      2      WIDTHL/WIDTHV)*(EXP(-0.4*CSPRD3**2.25) -10.0/
      3      (10.0+CSPRD3**2.25)))

      BRANCH=BRANCH +E
110   JI=JU+1.0
      JL=JL+1.0
      K=K+1.0
120   J=J+1.0

```

C SET FACTORS IN PREPARATION FOR THE NEXT BRANCH.

```

      BAND=BAND+BRANCH
      SYSTEM=SYSTEM+BRANCH
      K=KMIN
      IPRINT=IPRINT+2
      SWITCH= SWITCH+ 1

```

C GO TO THE APPROPRIATE BRANCH.

```

      GO TO (10,20,30,40,50,60,70,130), SWITCH

```

C COMPUTE APPROXIMATE BAND INTENSITY. SEE BATES, PAGE 57.

```

130   QR=TROT/(1.43879*BVU)
      APPROX=CINT2*QR*(NUBAR0**2*A0E)**2*EXP(-1.43879*CINT1+
      1      2.30259*CINT3)*2.0

      WRITE(6,601) (NAME(IPRINT,M1),M1=1,2),BRANCH,(FACTRI(M),M=1,5),
      1      BAND,(FACTRI(M),M=1,5),APPROX,(FACTRI(M),M=1,5)
      RETURN

```

C FORMATS FOR WRITE STATEMENTS.

```

600   FORMAT(94X,2A6,6HBRANCH ,4X,1PE10.4,5A1)
601   FORMAT(94X,2A6,8HBRANCHES,2X,1PE10.4,5A1//
      1      104X,10HBAND TOTAL,2X,1PE10.4,5A1/
      2      92X,22HAPPROXIMATE BAND TOTAL,2X,1PE10.4,5A1)
602   FORMAT(94X,2A6,8HBRANCHES,2X,1PE10.4,5A1)

```

END

\$\$\$ORIGIN ALPHA
 \$\$\$BFTC HF075H

SUBROUTINE ATOMIC

C SUBROUTINE ATOMIC COMPUTES THE ELECTRONIC TRANSITION FOR ATOMS.

```

      COMMON/CPLT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
      COMMON/CARRY/ILAM( 9000),ELAM( 9000)
      COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
      COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
      1      ALPHAL,BEL,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL,TERML
      COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,MU,ALTNAT,
      1      WEL,WEXEL,WEYEL,WEZEL,BVL,DVL, NUSPIN
      COMMON/CTEMP/TELECT,TVIB,TROT
      COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
      COMMON/CTRAN/PARTCC,NUBARO,Q,A0E,CINT1,CINT2,KMIN,KMAX
      COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

      REAL ILAM,LAMCL,LAMBDA,LAMMAX,LAMMIN,NAME
      DATA BLANK/6H /

```

C WRITE THE INTEGRATED INTENSITY FOR THE PREVIOUSLY COMPUTED SYSTEM.

```

      IF (SYSTEM.NE. 0.0) WRITE(6,600) SYSTEM,(FACTRI(M),M=1,5)
      TOTAL=TOTAL+SYSTEM
10    SYSTEM=0.0

      ATOMCC=READ1
      TELECT=READ2
      Q =READ3
      NAME=READ6

```

C WRITE THE GENERAL HEADING AND DATA FOR ATOMIC TRANSITIONS.

```

20    WRITE(6,601) READ6,ATOMCC,TELECT,Q

30    READ(5,500)WIDTHG,WIDTHL,DEGENU,TERMU,EINSTN,LAMCL,RANGE,READ6
      IF (READ6.EQ.BLANK) GO TO 50

```

C WRITE THE TOTAL INTEGRATED SPONTANEOUS EMISSION INTENSITY FOR THE
 C PRIOR ATOM.

```

WRITE(6,602) NAME,SYSTEM,(FACTRI(M),M=1,5)
NAME=READ6
SYSTEM=0.0
IF(TERMU .EQ. 0.0 .AND. DEGENU .NE. 0.0) GO TO 40
READ1=WIDTHG
READ2=WIDTHL
READ3=DEGENU
READ4=TERMU
READ5=EINSTN
RETURN

40  ATOMCC=WIDTHG
    TELECT= WIDTHL
    Q=DEGENU
    GO TO 20

C  FIND THE INTENSITY FACTOR, IF NECESSARY.

50  CINT1= TERMU/TELECT
    IFACR=0.62486*CINT1
    IF(IFACR .LT. 30) GO TO 90
    CINT4= IFACR
    IF(CINT4 .LT. CINT3) GO TO 90

    FACTRI(1)=OUTPUT(12)
    M=IFACR/1000
    DO 60 M1=2,5
        FACTRI(M1)=OUTPUT(M+1)
        IFACR=IFACR-M*10**(5-M1)
60  M=IFACR/10**(4-M1)

C  IF THIS IS NOT THE FIRST INTENSITY FACTOR, ADJUST THE ELAM ARRAY.

    IF(CINT3 .EQ. 0.0) GO TO 80
    CINT5= CINT4-CINT3
    DO 70 M=1,NARRAY
70  ELAM(M)=ELAM(M)*EXP(2.30259*CINT5)

    SYSTEM= SYSTEM*EXP(2.30259*CINT5)
    TOTAL= TOTAL*EXP(2.30259*CINT5)
80  CINT3= CINT4

C  RANGE IS THE DISTANCE FROM THE LINE CENTER, IN LINEWIDTHS, BEYOND WHICH THE
C  LINE INTENSITY IS CONSIDERED ZERO.

90  IF (RANGE .NE. 0.0) GO TO 95
    RANGE= 5.0
    IF (WIDTHL .EQ. 0.0) RANGE=3.0

C  FIND THE VOIGT LINE WIDTH AT HALF-HEIGHT.

95  WIDTHV=WIDTHL/2.0+SQRT(WIDTHL**2/4.0+WIDTHG**2)
    IF (WIDTHV .NE. 0.0) GO TO 100
    WIDTHV=10.0*DELLAM
    WIDTHG=WIDTHV
    WRITE(6,701)

C  FIND THE NUMBER OF ENTRIES IN THE INTENSITY ARRAY, FROM THE LINE CENTER,
C  AT WHICH EACH LINE IS ASSUMED TO HAVE A CONTRIBUTION.

100 NSPRD=1.1 +RANGE*WIDTHV/DELLAM

C  SET CONSTANTS WHICH DETERMINE THE LINE SHAPE.

    CSPRD2=WIDTHL/WIDTHV
    CSPRD3=(1.065+0.447*CSPRD2+0.058*CSPRD2**2)*WIDTHV*1.0E-4
    CSPRD1=(1.0-CSPRD2)/CSPRD3
    CSPRD2=CSPRD2/CSPRD3

C  IF THE LINE WAVELENGTH FALLS OUTSIDE THE SPECTRAL RANGE OF
C  INTEREST, OMIT IT AND PROCEED TO THE NEXT LINE.

    IF(LAMCL.LT.LAMMIN-RANGE*WIDTHV) GO TO 120
    IF(LAMCL.GT.LAMMAX+RANGE*WIDTHV) GO TO 120

C  FIND THE INTEGRATED LINE INTENSITY DUE TO SPONTANEOUS EMISSION.

    E=1.580E-16*ATOMCC*DEGENU*EINSTN*EXP(-1.43879*TERMU/TELECT
1    +2.30259*CINT3)/(Q*LAMCL)

C  SET CONSTANTS USED TO DISTRIBUTE THE ATOMIC LINE.

    NCENTR=1.5+(LAMCL-LAMMIN)/DELLAM
    NSTART=NCENTR-NSPRD
    IF (NSTART .LT. 1) NSTART=1
    NEND=NCENTR +NSPRD
    IF (NEND .GT. NARRAY) NEND=NARRAY

C  DISTRIBUTE THE ATOMIC LINE.

    DO 110 M1=NSTART,NEND
        COUNT=M1
        LAMBDA=LAMMIN +(COUNT-1.0)*DELLAM
        CSPRD3=ABS((LAMBDA-LAMCL)/WIDTHV)
110  ELAM(M1)=ELAM(M1) +E*(CSPRD1*EXP(-2.772*CSPRD3**2)
1      +CSPRD2/(1.0+4.0*CSPRD3**2) +0.016* CSPRD2*(1.0-
2      WIDTHL/WIDTHV)*(EXP(-0.4*CSPRD3**2.25) -10.0/
3      (10.0+CSPRD3**2.25)))

```

```

      SYSTEM=SYSTEM+E
      TOTAL=TOTAL+E

C PRINT ATOMIC LINE INFORMATION.

      IDEGEN= DEGENU+ 0.1
      IRANGE= RANGE+ 0.1
      WRITE(6,603) LAMCL,IDEGEN,TERMU,EINSTN,WIDTHG,WIDTHL,WIDTHV,
1      IRANGE,E,(FACTRI(M),M=1,5)
      GO TO 30

C LINE WAVELENGTH FALLS OUTSIDE SPECTRAL RANGE OF INTEREST.

120  WRITE(6,700) LAMCL
      GO TO 30

C FORMAT FOR READ STATEMENT.

500  FORMAT(6E10.0,E6.0,A6)

C FORMATS FOR WRITE STATEMENTS.

600  FORMAT(/103X,12HSYSTEM TOTAL,1X,1PE10.4,5A1)
601  FORMAT(/52X,25HATOMIC LINE SPECTRUM FOR ,A6//
1      35X,9HNUMBER OF/
1      35X,5HATOMS,20X,
1      10HELECTRONIC,16X,9HPARTITION/
2      35X,6HPER CC,19X,11HTEMPERATURE,15X,8HFUNCTION//
3      35X,1PE10.4,15X,E10.4,16X,E10.4//
4      9X,10HWAVELENGTH,6X,10HELECTRONIC,6X,10HELECTRONIC,6X,
5      8HEINSTEIN,9X,11HATOMIC LINE,16X,5H RANGE,10X,10HINTEGRATED/
6      9X,12HIN ANGSTROMS,4X,10HDEGENERACY,6X,11HTERM ENERGY,
7      5X,7HA COEFF,10X,20HWIDTH AT HALF-HEIGHT,7X,7HIN LINE,
8      8X,9HINTENSITY/
9      74X,21HGAUSS LORENTZ VOIGT,6X,6HWIDTHS,9X,8HW/CM2-SR//)
602  FORMAT(/76X,10HSUM OF THE,1X,A6,1X,21HATOMIC LINES INCLUDED,
1      1X,1PE10.4,5A1)
603  FORMAT(9X,F9.3,11X,I2,10X,1PE11.5,5X,1PE10.4,5X,3(OPF7.3,1X),
1      5X,I4,11X,1PE10.4,5A1)

C FORMATS FOR ERROR STATEMENTS.

700  FORMAT( 10X,8HLINE AT,1PE10.4,43H ANGSTROMS FALLS OUTSIDE THE PLOT
      1TING RANGE)
701  FORMAT(/8X,117HLINE WIDTHS WERE NOT INPUT FOR NEXT LINE. PROGRAM I
      1MPOSED A GAUSSIAN PROFILE WITH WIDTH AT HALF-HEIGHT = 10*INTERVAL.
      2)

      END
*****

$ORIGIN      ALPHA
$IBFTC HF075J

      SUBROUTINE PRINT(NEWCAS)

C SUBROUTINE PRINT TABULATES SPECTRAL INTENSITY VS WAVELENGTH ON THE
C WRITTEN OUTPUT.

C IN THIS SUBROUTINE, THE ILAM ARRAY, WHICH NOW CONTAINS WAVELENGTHS, WILL
C BE NAMED LAMBDA.

      COMMON/CPLLOT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
      COMMON/CARRAY/LAMBDA( 9000),ELAM(9000)
      COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
      COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
1      ALPHAL,BEL,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL,TERML
      COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,MU,ALTNAT,
1      WEL,WEXEL,WEYEL,WEZEL,BVL,DVL,      NUSPIN
      COMMON/CTEMP/TELECT,TVIB,TROT
      COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
      COMMON/CTRAN/PARTCC,NUBARO,Q,AOE,CINT1,CINT2,KMIN,KMAX
      COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

      REAL LAMBDA,LAMMAX,LAMMIN
      LOGICAL NEWCAS
      DATA LOG/6HLOG

C WRITE GENERAL HEADING AND READ A CARD SPECIFYING WHETHER THE
C INTENSITIES ARE TO BE PRINTED AS LINEAR OR LOG VALUES.

      WRITE(6,600)
      IF(NEWCAS) GO TO 50
      READ (5,500) KIND
      IF(KIND .NE. LOG) GO TO 50

C A LOG OUTPUT IS DESIRED.

C WRITE HEADING FOR THE LOG OUTPUT, ENSURE THAT THE LOG OF ZERO WILL
C NOT BE TAKEN, AND APPLY THE INTENSITY FACTOR.

      WRITE(6,601)
      DO 10 M=1,NARRAY
      IF (ELAM(M) .EQ. 0.0) ELAM(M)=1.0E-38
10      ELAM(M)=ALOG10(ELAM(M)) - CINT3

```

```

      NWRITE=NARRAY/4
      N1=NWRITE+1
      N2=2*NWRITE+1
      N3=3*NWRITE+1

C   PRINT THE LAMBDA VERSUS LOG(ELAM) VALUES IN FOUR COLUMNS ACROSS THE PAGE.

      DO 20 M=1,NWRITE
        WRITE(6,602) LAMBDA(M),ELAM(M),LAMBDA(N1),ELAM(N1),LAMBDA(N2),
1          ELAM(N2),LAMBDA(N3),ELAM(N3)
        N1=N1+1
        N2=N2+1
20      N3=N3+1

C   IS THE PRINTING COMPLETED. IF SO, RETURN TO THE MAIN PROGRAM.

      IF (4*NWRITE.EQ.NARRAY) RETURN
      N1=4*NWRITE+1
      NWRITE=NARRAY-4*NWRITE

C   WRITE THE REMAINING VALUES AND RETURN TO THE MAIN PROGRAM.

      DO 30 M=1,NWRITE
        WRITE(6,603) LAMBDA(N1),ELAM(N1)
30      N1=N1+1
        RETURN

C   A LINEAR OUTPUT IS DESIRED.

C   WRITE THE HEADING FOR THE LINEAR OUTPUT.

50      WRITE(6,605)
      NWRITE=NARRAY/4
      N1=NWRITE+1
      N2=2*NWRITE+1
      N3=3*NWRITE+1

C   PRINT THE LAMBDA VERSUS ELAM VALUES IN FOUR COLUMNS ACROSS THE PAGE.

      DO 60 M=1,NWRITE
        WRITE(6,606) LAMBDA(M),ELAM(M),(FACTRI(M),M1=1,5),LAMBDA(N1),
1          ELAM(N1),(FACTRI(M1),M1=1,5),LAMBDA(N2),ELAM(N2),
2          (FACTRI(M1),M1=1,5),LAMBDA(N3),ELAM(N3),
3          (FACTRI(M1),M1=1,5)
        N1=N1+1
        N2=N2+1
60      N3=N3+1

C   IS THE PRINTING COMPLETED. IF SO, RETURN TO THE MAIN PROGRAM.

      IF (4*NWRITE.EQ.NARRAY) RETURN
      N1=4*NWRITE+1
      NWRITE=NARRAY-4*NWRITE

C   WRITE THE REMAINING VALUES AND RETURN TO THE MAIN PROGRAM.

      DO 70 M=1,NWRITE
        WRITE(6,607) LAMBDA(N1),ELAM(N1),(FACTRI(M1),M1=1,5)
70      N1=N1+1
        RETURN

C   FORMAT FOR READ STATEMENT.

500      FORMAT(66X,A6)

C   FORMATS FOR WRITE STATEMENTS.

600      FORMAT(//49X,34HTABULATION OF COMPUTED SPECTRUM//)
601      FORMAT(4(3X,29HWAVELENGTH LOG 10(INTENSITY,1X)/
1          4(3X,29HANGSTROMS W/CM2-MICRON-SR),1X)///)
602      FORMAT(4(4X,F8.2,5X,F10.4,6X))
603      FORMAT(103X,F8.2,5X,F10.4)
605      FORMAT(4(3X,21HWAVELENGTH INTENSITY,8X)/
1          4(3X,27HANGSTROMS W/CM2-MICRON-SR,2X)///)
606      FORMAT(4(4X,0PF8.2,4X,1PE11.4,5A1))
607      FORMAT(100X,F8.2,4X,1PE11.4,5A1)

      END

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$ORIGIN      ALPHA
$IBFTC HF075K

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      SUBROUTINE INTRVL(NINTRV)

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C   SUBROUTINE INTRVL COMPUTES INTEGRATED INTENSITIES BETWEEN SPECIFIED
C   WAVELENGTHS.

C   IN THIS SUBROUTINE, THE ILAM ARRAY, WHICH NOW CONTAINS WAVELENGTHS, WILL
C   BE NAMED LAMBDA.

      COMMON/CPLLOT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
      COMMON/CARRAY/LAMBDA( 9000),ELAM( 9000)
      COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
      COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
1          ALPHAL,BEL,BETAL,CAPAL,CAPLU,DEL,DZEROL,REL,TERML
      COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,MU,ALTNAT,
1          WEL,WEXEL,WEYEL,WEZEL,BVL,DVL,          NUSPIN

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COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
COMMON/CTRAN/PARTCC,NUBARO,Q,AOE,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

REAL LAM1,LAM2,LAMMAX,LAMMIN,LAMBDA,

C WRITE GENERAL HEADING AND READ WAVELENGTH LIMITS FOR INTEGRATION
C INTERVAL.

WRITE(6,600)
10 READ(5,500) LAM1, LAM2

C INITIALIZE INTEGRATED INTENSITY FOR THIS INTERVAL.

TOTALI=0.0

C IF THE UPPER WAVELENGTH LIMIT WAS INPUT FIRST, WRITE AN ERROR
C MESSAGE AND OMIT THIS INTERVAL.

IF (LAM2 .LE. LAM1) GO TO 70

C IF WAVELENGTH LIMITS ARE OUTSIDE SPECTRAL RANGE CONSIDERED, SET
C INTEGRATION LIMITS TO APPROPRIATE END WAVELENGTH.

IF (LAM1 .LT. LAMMIN) LAM1=LAMMIN
IF (LAM2 .GT. LAMMAX) LAM2=LAMMAX

C FIND INDICES IN INTENSITY ARRAY TO BE INCLUDED IN INTEGRATION.

NSTART= 1.0 +(LAM1-LAMMIN)/DELLAM
NEND= 1.0 +(LAM2-LAMMIN)/DELLAM

C TEST INTERVAL LIMITS.

IF (NSTART .LT. NEND) GO TO 20

C THE INTERVAL IS BOUNDED BY CONSECUTIVE ENTRIES IN THE LAMBDA ARRAY.

SLOPE=(ELAM(NSTART+1)-ELAM(NSTART))/DELLAM
TOTALI=((SLOPE*(LAM1-LAMBDA(NSTART))+ELAM(NSTART))+(SLOPE*(LAM2-
1 LAMBDA(NSTART))+ELAM(NSTART)))*(LAM2-LAM1)/2.0E+4
GO TO 50

C IS THERE A RIGHT-HAND INCREMENT.

20 IF (NEND.EQ.NARRAY) GO TO 30

C COMPUTE INTEGRATED INTENSITY FROM RIGHT-HAND INCREMENTAL AREA.

ELAM1=(ELAM(NEND+1)-ELAM(NEND))*(LAM2-LAMBDA(NEND))/
1 DELLAM+ELAM(NEND)
TOTALI=(ELAM1+ELAM(NEND))*(LAM2-LAMBDA(NEND))/2.0E+4

C COMPUTE INTEGRATED INTENSITY FROM LEFT-HAND INCREMENTAL AREA.

30 ELAM1=(ELAM(NSTART)-ELAM(NSTART+1))*(LAMBDA(NSTART+1)-LAM1)/
1 DELLAM+ELAM(NSTART+1)
TOTALI=TOTALI+(ELAM1+ELAM(NSTART+1))*(LAMBDA(NSTART+1)-LAM1)/2.E+4

C DO INTERVAL LIMITS BOUND A SINGLE ENTRY IN THE LAMBDA ARRAY.

IF (NEND .EQ. NSTART+1) GO TO 50

C COMPUTE INTEGRATED INTENSITY FROM CENTRAL INCREMENTAL AREAS.

NSTART=NSTART+2
DO 40 M=NSTART,NEND
40 TOTALI=TOTALI+(ELAM(M)+ELAM(M-1))*DELLAM/2.0E+4

C WRITE WAVELENGTH LIMITS AND RESULTING VALUE OF INTEGRATION.

50 WRITE(6,601) LAM1,LAM2,TOTALI,(FACTRI(M),M=1,5)

C IF INTEGRATION HAS BEEN COMPLETED FOR ALL SPECIFIED INTERVALS,
C RETURN TO MAIN PROGRAM.

60 NINTRV=NINTRV-1
IF (NINTRV.NE.0) GO TO 10
RETURN

C THERE IS AN ERROR IN THE LIMITS FOR THE INTEGRATION INTERVAL.

70 WRITE(6,700) LAM1,LAM2
GO TO 60

C FORMAT FOR READ STATEMENT.

500 FORMAT(2E10.0)

C FORMATS FOR WRITE STATEMENTS.

600 FORMAT(///50X,31HINTEGRATED SPECTRAL INTENSITIES//
1 35X,16HLOWER WAVELENGTH 10X,16HUPPER WAVELENGTH,10X,10HINTEGR
2ATED/ 35X,5HLIMIT 21X,5HLIMIT,21X,9HINTENSITY/
3 35X,9HANGSTROMS17X,9HANGSTROMS,17X,8HW/CM2-SR//)
601 FORMAT(35X,1PE10.4,16X,E10.4,16X,E10.4,5A1)

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C FORMAT FOR ERROR STATEMENT.

700 FORMAT(/10X,16HTHE LOWER LIMIT ,1PE11.4,33H IS GREATER THAN THE U
PPER LIMIT ,E11.4,36H THUS INTEGRATION WAS NOT PERFORMED.)

END

\$ORIGIN ALPHA
\$IBFTC HF075L

SUBROUTINE SLIT(NSLIT)

C SUBROUTINE SLIT COMPUTES THE OUTPUT SIGNAL GIVEN BY A SPECIFIED
C INSTRUMENT SENSITIVITY.

C IN THIS SUBROUTINE, THE ILAM ARRAY, WHICH NOW CONTAINS WAVELENGTHS, WILL
C WILL BE NAMED LAMBDA.

COMMON/CPLT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/LAMDA(9000),ELAM(9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
1 ALPHAL,BEL,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL,TERML
COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,MU,ALTNAT,
1 WEL,WEXEL,WEYEL,WEZEL,BVL,DVL, NUSPIN
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CWIDTH/WIDTHL,WIDTHH,RANGE
COMMON/CTRAN/PARTCC,NUBARO,Q,AOE,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

DIMENSION LAM(100),RSLIT(100),LAMR(100),RLAM(100),LAMS(500),
1SIGLAM(500),LAMSAV(100)
REAL LAM1,LAM2,LAM,LAMBDA,LAMR,LAMS,LAMCL,LAMS1,LAMS2,LAMSAV
INTEGER BLOCK,FACTRI,SCAN,FLAG
DATA SLIT1/4HSLIT/

C WRITE THE GENERAL HEADING AND INITIALIZE THE COUNTER SPECIFYING
C HOW MANY SLIT CASES HAVE BEEN COMPLETED.

WRITE(6,600)
MSLIT=0

C ARE ALL THE DESIRED SLIT CASES COMPLETED. IF SO, RETURN TO THE MAIN PROGRAM.

5 IF(MSLIT.EQ.NSLIT) RETURN

C THIS IS THE STARTING POINT FOR THE CONSIDERATION OF EACH NEW SLIT CASE.

C IF AN ERROR WAS DETECTED IN THE PRIOR CASE, READ THROUGH THE REMAINING CARDS.

6 READ(5,505) SEARCH
IF(SEARCH.NE.SLIT1) GO TO 6
MSLIT=MSLIT+1

C INITIALIZE THE INSTRUMENT OUTPUT SIGNAL.

SIGNAL=0.0
WRITE(6,616)

C READ THE CARD THAT SPECIFIES THE TYPE OF INSTRUMENT SENSITIVITY TO BE
C CONSIDERED.

C NPOINT= NUMBER OF ARRAY ELEMENTS SPECIFYING SLIT FUNCTION. IF
C NPOINT=0, THE SLIT FUNCTION IS SPECIFIED BY A GAUSSIAN CURVE.
C SCAN= 1 SPECIFIES A SCANNING SLIT CASE. SCAN= 0 SPECIFIES A FIXED
C SLIT CASE.
C STEP= DISTANCE IN ANGSTROMS THAT THE SLIT IS MOVED FOR EACH STEP OF
C THE SCAN.
C LAMS1= STARTING WAVELENGTH OF THE SCAN FOR A SCANNING SLIT. LOCATION
C OF THE SLIT CENTER LINE FOR A FIXED LINEAR SLIT.
C LAMS2= STOPPING WAVELENGTH OF THE SCAN FOR A SCANNING SLIT.
C NRLAMS= NUMBER OF ARRAY ELEMENTS IN THE SPECTRAL CALIBRATION ARRAY.

READ(5,500) NPOINT,SCAN,STEP,LAMS1,LAMS2,NRLAMS

C WRITE HEADINGS FOR THE APPROPRIATE CASE.

IF(SCAN.NE.1) WRITE(6,601) MSLIT
IF(SCAN.EQ.1) WRITE(6,602) MSLIT,LAMS1,LAMS2,STEP

C WAS THE UPPER SCAN LIMIT INPUT LESS THAN OR EQUAL TO THE LOWER LIMIT.
C IF SO, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.

IF(SCAN.EQ.1.AND.LAMS2.LE.LAMS1) GO TO 272

C IS THE SLIT FUNCTION SPECIFIED BY A GAUSSIAN CURVE OR BY A SET
C OF LINEAR SEGMENTS.

IF(NPOINT.EQ.0) GO TO 25

C THE SLIT FUNCTION IS SPECIFIED BY LINEAR SEGMENTS. READ IN,
C PRINT, AND TEST THE DEFINING VALUES OF THE SLIT FUNCTION.

READ(5,502) (LAM(M),RSLIT(M),M=1,NPOINT)
WRITE(6,603)
WRITE(6,604) (LAM(M),RSLIT(M),M=1,NPOINT)

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C DO THE WAVELENGTHS SPECIFYING THE SLIT FUNCTION INCREASE
C MONOTONICALLY. IF NOT, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.

      M1=NPOINT-1
      DO 10 M=1,M1
        IF(LAM(M).GE.LAM(M+1)) GO TO 265
10     CONTINUE

C FIND THE PEAK OF THE SLIT FUNCTION AND COMPUTE THE EFFECTIVE WIDTH OF THE
C SLIT FUNCTION SPECIFIED BY LINEAR SEGMENTS.

      WIDTH=0.0
      RMAX=0.0
      DO 15 M=1,NPOINT
        IF(RSLIT(M).GT.RMAX) RMAX=RSLIT(M)
15     M1=NPOINT-1
      DO 20 M=1,M1
        WIDTH=WIDTH+0.5*(RSLIT(M+1)+RSLIT(M))*(LAM(M+1)-LAM(M))/RMAX
20

C READ THE DATA DENOTING THE CENTER OF THE SLIT FUNCTION AND THE CALIBRATION
C FACTOR USED TO SPECIFY THE INSTRUMENT SENSITIVITY IF THIS IS A FIXED
C WAVELENGTH RADIOMETER.

      READ(5,503) LAMCL,RLAMCL

C IS THE SPECIFIED CENTER OF THE SLIT FUNCTION COMPATIBLE WITH THE SLIT
C FUNCTION DATA. IF NOT, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.

      IF(LAMCL.LT.LAM(1).OR.LAMCL.GT.LAM(NPOINT)) GO TO 266
      GO TO 30

C THE SLIT FUNCTION IS SPECIFIED BY A GAUSSIAN FUNCTION. PRINT THE
C HEADING AND READ THE DEFINING DATA.

25  WRITE(6,607)
      READ(5,501) LAMCL,RLAMCL,WIDTH

C IS THIS A SPECTROGRAPH OR SCANNING SPECTROMETER CASE.

30  IF(SCAN.EQ.1) GO TO 45

C THIS IS A FIXED WAVELENGTH RADIOMETER.

      IF(NPOINT.EQ.0) GO TO 40

C PRINT ADDITIONAL LINEAR SLIT DATA.

      WRITE(6,605) LAMCL,LAMS1,RLAMCL,WIDTH

C POSITION THE SLIT AT THE SPECIFIED WAVELENGTH.

      SHIFT=LAMS1-LAMCL
      DO 35 M=1,NPOINT
        LAM(M)=LAM(M)+SHIFT
35

C IF PART OR ALL OF THE INSTRUMENT SENSITIVITY LIES OUTSIDE THE
C COMPUTED SPECTRUM, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.

      IF(LAM(1).LT.LAMBDA(1)) GO TO 260
      IF(LAM(NPOINT).GT.LAMBDA(NARRAY)) GO TO 260
      GO TO 125

C PRINT THE GAUSSIAN INPUT DATA.

40  WRITE(6,608) LAMCL,RLAMCL,WIDTH
      TEST1=LAMBDA(1)-(LAMCL-3.0*WIDTH)
      IF(TEST1.GT.0.0) GO TO 260
      TEST2=LAMBDA(NARRAY)-(LAMCL+3.0*WIDTH)
      IF(TEST2.LT.0.0) GO TO 260
      GO TO 155

C THIS IS A SPECTROGRAPH OR A SCANNING SPECTROMETER CASE. POSITION THE
C SLIT AT THE START OF THE SCAN AND TEST THE SPECIFIED END POINTS OF
C THE DESIRED SPECTRAL COVERAGE.

45  IF(NPOINT.EQ.0) GO TO 70

C THE SLIT FUNCTION IS SPECIFIED BY A LINEAR SLIT.
C PRINT ADDITIONAL SLIT DATA.

      WRITE(6,606)
      WRITE(6,604) LAMCL,WIDTH

C POSITION THE LINEAR SLIT AT THE SPECIFIED STARTING WAVELENGTH FOR THE SCAN.

      SHIFT=LAMS1-LAMCL
      DO 55 M=1,NPOINT
        LAM(M)=LAM(M)+SHIFT
55

C TEST THE INPUT DATA FOR THE LINEAR SCANNING SLIT.
C IF PART OR ALL OF THE INSTRUMENT SENSITIVITY WILL FALL OUTSIDE THE
C COMPUTED SPECTRUM, MAKE THE APPROPRIATE ADJUSTMENT AND WRITE A MESSAGE
C INDICATING THIS WAS DONE.

      TEST1=LAMBDA(1)-LAM(1)
      IF(TEST1.LE.0.0) GO TO 65
      LAMS1=LAMS1+TEST1
      DO 60 M=1, NPOINT

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60     LAM(M)=LAM(M) + TEST1
65     TEST2=LAMBDA(NARRAY)-(LAMS2+LAM(NPOINT)-LAMS1)
      GO TO 77
C     PRINT THE GAUSSIAN SLIT DATA.
70     WRITE(6,609) WIDTH
C     TEST THE INPUT DATA FOR THE GAUSSIAN SCANNING SLIT.
C     IF PART OR ALL OF THE INSTRUMENT SENSITIVITY WILL FALL OUTSIDE THE
C     COMPUTED SPECTRUM, MAKE THE APPROPRIATE ADJUSTMENT AND WRITE A MESSAGE
C     INDICATING THIS WAS DONE.
      TEST1=LAMBDA(1)-(LAMS1-3.0*WIDTH)
      IF(TEST1.LE.0.0) GO TO 75
      LAMS1=LAMS1+TEST1
75     TEST2=LAMBDA(NARRAY)-(LAMS2+3.0*WIDTH)
77     IF(TEST2.LT.0.0) LAMS2=LAMS2+TEST2
      IF(TEST1.GT.0.0.OR.TEST2.LT.0.0) WRITE(6,702) LAMS1,LAMS2,STEP
C     POSITION THE SLIT AT THE SPECIFIED STARTING WAVELENGTH OF THE SCAN.
      LAMCL=LAMS1
C     READ AND PRINT DATA SPECIFYING SPECTRAL CALIBRATION OF SCANNING SLIT.
      READ(5,502)(LAMR(M),RLAM(M),M=1,NRLAMS)
      WRITE(6,610)
      WRITE(6,604)(LAMR(M), RLAM(M),M=1,NRLAMS)
C     IF THE WAVELENGTH VALUES OF THE SPECTRAL CALIBRATION DO NOT INCREASE
C     MONOTONICALLY, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.
      M2=NRLAMS-1
      DO 90 M=1,M2
        IF(LAMR(M).GE.LAMR(M+1)) GO TO 270
90     CONTINUE
C     IF THE END POINTS OF THE SPECTRAL CALIBRATION DO NOT BOUND THE
C     SCANNING RANGE, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.
      IF(LAMS1.LT.LAMR(1)) GO TO 271
      IF(LAMS2.GT.LAMR(NRLAMS)) GO TO 271
C     SET THE INITIAL VALUES OF COUNTERS AND WAVELENGTHS FOR THE SCAN.
      NSIGLM=1
      LAMS(1)=LAMS1
      BLOCK=1
      FLAG=0
      NSTEP=0
C     THIS IS THE STARTING POINT FOR EACH STEP OF THE SCAN.
C     LOCATE THE SLIT CENTER WAVELENGTH BETWEEN THE PROPER ELEMENTS IN
C     THE SPECTRAL CALIBRATION ARRAY.
      NRLAM=1
95     IF(LAMCL.GE.LAMR(NRLAM).AND.LAMCL.LE.LAMR(NRLAM+1)) GO TO 115
      NRLAM= NRLAM+1
      GO TO 95
C     FIND THE SPECTRAL CALIBRATION RLAMCL AT THE SLIT CENTER FOR THIS
C     STEP OF THE SCAN.
115    RLAMCL=RLAM(NRLAM)+(LAMCL-LAMR(NRLAM))*(RLAM(NRLAM+1)-
      1RLAM(NRLAM))/(LAMR(NRLAM+1)-LAMR(NRLAM))
      IF(NPOINT.EQ.0) GO TO 155
C     THE INTEGRATION SCHEME FOR LINEAR SLITS BEGINS HERE.
C     SET THE INITIAL INDEX VALUES FOR THE INTEGRATION. N1 AND N2 ARE
C     INDICES IN THE SPECTRAL ARRAY. M1 AND M2 ARE INDICES IN THE
C     SLIT FUNCTION ARRAY.
125    NSTART=1.1+(LAM(1)-LAMBDA(1))/DELLAM
      N1=NSTART
      N2=N1+1
      M1=1
      M2=2
C     COMPUTE THE SPECTRAL INTENSITY AT THE LEFT-HAND END POINT OF
C     THE SLIT FUNCTION.
      LAM1=LAM(1)
      RSLIT1=RSLIT(1)
      ELAM1=ELAM(N2) +(LAMBDA(N2)-LAM(1))*(ELAM(N1)-ELAM(N2))/
      1      DELLAM
C     IS THE RIGHT-HAND POINT OF THE INTERVAL IN THE SPECTRUM OR SLIT
C     FUNCTION ARRAY.
135    IF(LAMBDA(N2).LT.LAM(M2)) GO TO 140

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C THE RIGHT-HAND POINT OF THE INTERVAL IS IN THE SLIT FUNCTION ARRAY.
    LAM2=LAM(M2)
    RSLIT2=RSLIT(M2)
    ELAM2=ELAM(N2) + (LAMBDA(N2)-LAM(M2))*(ELAM(N1)-ELAM(N2))/
1    DELLAM
    M1=M1+1
    M2=M2+1
    GO TO 145

C THE RIGHT-HAND POINT OF THE INTERVAL IS IN THE SPECTRUM ARRAY.
140  LAM2=LAMBDA(N2)
    RSLIT2=RSLIT(M2)+(LAM(M2)-LAMBDA(N2))*(RSLIT(M1)-RSLIT(M2))/
1    (LAM(M2)-LAM(M1))
    ELAM2=ELAM(N2)
    N1=N1+1
    N2=N2+1

C GENERATE THE LINEAR SLIT INSTRUMENT OUTPUT SIGNAL.
145  SIGNAL=SIGNAL +(ELAM1*RSLIT1+ELAM2*RSLIT2)*RLAMCL*
1    (LAM2-LAM1)/2.0E+4

C IS THE INTEGRATION FOR THIS SLIT OR THIS STEP IN THE SCAN COMPLETE.
    IF (LAM(NPOINT)-LAM2.LE.0.1*DELLAM) GO TO 150

C MOVE TO THE NEXT INTERVAL.
C THE LEFT-HAND POINT OF THE NEW INTERVAL IS THE RIGHT-HAND POINT OF
C THE PRIOR INTERVAL.
    LAM1=LAM2
    RSLIT1=RSLIT2
    ELAM1=ELAM2
    GO TO 135

C DIVIDE BY THE SLIT WIDTH TO YIELD THE INSTRUMENT OUTPUT
C AT THIS WAVELENGTH.
150  SIGNAL=SIGNAL/(WIDTH*1.0E-04)
    GO TO 165

C THE INSTRUMENT SENSITIVITY IS SPECIFIED BY A GAUSSIAN CURVE.
C THE INTEGRATION SCHEME FOR GAUSSIAN SLITS BEGINS HERE.
C FIND INDICES IN THE SPECTRUM ARRAY TO BE INCLUDED IN THE INTEGRATION.
155  NSTART=1.1+(LAMCL-3.0*WIDTH-LAMBDA(1))/DELLAM
    NEND=6.0*WIDTH/DELLAM
    NEND=NSTART+NEND+1

C SET THE INITIAL INDEX VALUES FOR THE INTEGRATION.
    N1=NSTART
    N2=N1+1

C COMPUTE THE PRODUCT OF SPECTRAL INTENSITY AND INSTRUMENT SENSITIVITY
C AT THE LEFT-HAND SIDE OF THE INTEGRATION ELEMENT.
    ELAM1=ELAM(N1)*RLAMCL*EXP(-2.772*((LAMBDA(N1)-LAMCL)/WIDTH)**2)

C COMPUTE THE PRODUCT OF SPECTRAL INTENSITY AND INSTRUMENT SENSITIVITY AT
C THE RIGHT-HAND SIDE OF THE INTEGRATION ELEMENT.
160  ELAM2=ELAM(N2)*RLAMCL*EXP(-2.772*((LAMBDA(N2)-LAMCL)/WIDTH)**2)

C GENERATE THE GAUSSIAN SLIT INSTRUMENT OUTPUT SIGNAL.
    SIGNAL=SIGNAL +(ELAM1+ELAM2)*DELLAM/2.0E+04
    N1=N1+1
    N2=N2+1

C IS THE INTEGRATION FOR THIS SLIT OR THIS STEP IN THE SCAN COMPLETE.
    IF (N2 .GT. NEND) GO TO 161
    ELAM1=ELAM2
    GO TO 160

C DIVIDE BY THE APPROPRIATE SLIT WIDTH TO YIELD THE INSTRUMENT OUTPUT
C AT THIS WAVELENGTH.
161  SIGNAL=SIGNAL/(WIDTH*1.06439E-04)

C IS THIS A SCANNING SLIT CASE.
165  IF (SCAN .NE. 1) GO TO 255

C THIS IS A SCANNING SLIT CASE.
    SIGLAM(NSIGLM)=SIGNAL

C IS THE SCAN COMPLETED.
    IF (FLAG.EQ.1) GO TO 250

C IS A DATA BLOCK CONTAINING 500 ENTRIES FROM THIS SCAN COMPLETED. IF SO, GO
C TO THE PORTION OF THE SUBROUTINE WHERE THE DATA BLOCK WILL BE PRINTED ON
C THE OUTPUT SHEET.
    IF (NSIGLM.EQ.500) GO TO 250

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C IS THE NEXT STEP THE LAST FOR THIS SCAN.

180  TEST=LAMS2-LAMS(NSIGLM)
    IF(TEST.LE.STEP) GO TO 200

C SET THE COUNTERS AND WAVELENGTHS FOR THE NEXT STEP OF THE SCAN.
    NSTEP=NSTEP+1
    COUNT=NSTEP
    LAMCL=LAMS1+COUNT*STEP

C IF A DATA BLOCK WAS JUST PRINTED (NSIGLM=500), READJUST THE COUNTER NSIGLM.
    IF(NSIGLM.NE.500) GO TO 185
    NSIGLM=1
    LAMS(1)=LAMS1+COUNT*STEP
    GO TO 190

185  NSIGLM=NSIGLM+1
    LAMS(NSIGLM)=LAMS1+COUNT*STEP

190  IF(NPOINT.EQ.0) GO TO 225

C SAVE THE WAVELENGTHS OF THE SLIT FUNCTION AT THE FIRST SCANNING LOCATION.
    IF(NSTEP.GT.1) GO TO 196
    DO 195 M=1,NPOINT
195  LAMSAV(M)=LAM(M)
196  DO 197 M=1,NPOINT
197  LAM(M)=LAMSAV(M)+COUNT*STEP
    GO TO 225

C SET UP THE LAST STEP OF THE SCAN.

200  FLAG=1
    LAMCL=LAMS2

C IF A DATA BLOCK WAS JUST PRINTED, READJUST THE COUNTER NSIGLM.
    IF(NSIGLM.NE.500) GO TO 205
    NSIGLM=1
    LAMS(1)=LAMS2
    GO TO 210

205  NSIGLM=NSIGLM+1
    LAMS(NSIGLM)=LAMS2

210  IF(NPOINT.EQ.0) GO TO 225
    DO 215 M=1, NPOINT
215  LAM(M)=LAM(M)+TEST

C RE-INITIALIZE SIGNAL FOR THE NEXT STEP OF THE SCAN.

225  SIGNAL=0.0
    GO TO 95

C IF THIS IS THE FIRST DATA BLOCK, PRINT THE SCAN DATA HEADING ON THE
C OUTPUT SHEET.

250  IF(BLOCK.EQ.1) WRITE(6,612)

C PRINT THE SCAN DATA ON THE OUTPUT SHEET.
    WRITE(6,613) (LAM(M),SIGLAM(M),(FACTRI(M),M=1,5), M=1,NSIGLM)

C IS THIS SCAN CASE COMPLETED.
    IF(FLAG.EQ.1) GO TO 5

C THE SCAN CASE IS NOT COMPLETED. CONTINUE THE SCAN.
    BLOCK=BLOCK+1
    GO TO 180

C WRITE THE FIXED WAVELENGTH RADIOMETER DATA ON THE OUTPUT SHEET.

255  WRITE(6,615) SIGNAL,(FACTRI(M),M=1,5)
    GO TO 5

C THERE IS AN ERROR IN THE SLIT INPUT DATA. WRITE AN ERROR MESSAGE
C AND CONTINUE.

C ALL OR PART OF THE FIXED SLIT LIES OUTSIDE THE COMPUTED SPECTRUM.

260  WRITE(6,700)
    GO TO 5

C WAVELENGTHS SPECIFYING THE LINEAR SLIT FUNCTION DO NOT INCREASE
C MONOTONICALLY.

265  WRITE(6,701)
    GO TO 5

C SPECIFIED CENTER OF THE SLIT FUNCTION LIES OUTSIDE THE SPECIFIED SLIT
C FUNCTION.

```

```

266  WRITE(6,606)
      WRITE(6,604) LAMCL,WIDTH
      WRITE(6,704)
      GO TO 5

C  WAVELENGTHS OF SPECTRAL CALIBRATION DO NOT INCREASE MONOTONICALLY.

270  WRITE(6,701)
      GO TO 5

C  WAVELENGTHS SPECIFYING THE SPECTRAL CALIBRATION
C  DO NOT BOUND THE DESIRED SCAN RANGE.

271  WRITE(6,703)
      GO TO 5

C  UPPER SCAN LIMIT WAS INPUT LESS THAN OR EQUAL TO THE LOWER LIMIT.

272  WRITE(6,705)
      GO TO 5

C  FORMATS FOR READ STATEMENTS.

500  FORMAT(15,4X,11,4X,3E10.0,1X,15)
501  FORMAT(3E10.0)
502  FORMAT(6E10.0)
503  FORMAT(2E10.0)
504  FORMAT(2E13.7)
505  FORMAT(1A4)

C  FORMATS FOR WRITE STATEMENTS.

600  FORMAT(////
1      34X,63HDETECTOR OUTPUT SIGNAL GIVEN BY A SPECIFIED INSTRUME
2NT RESPONSE////)
601  FORMAT(49X, 27HFIXED WAVELENGTH RADIOMETER,2X,13//)
602  FORMAT(42X, 37HSPECTROGRAPH OR SCANNING SPECTROMETER,2X,13//
118X,20HSPECTRAL RANGE FROM ,F8.2,4H TO ,F8.2,23H ANGSTROMS COMPUTE
2D AT ,F6.3,19H ANGSTROM INTERVALS//)
603  FORMAT(42X,42HSLIT FUNCTION SPECIFIED BY LINEAR SEGMENTS//
1      50X,10HWAVELENGTH,11X,4HSLIT/
2      50X, 9HANGSTROMS ,12X,8HFUNCTION//)
604  FORMAT(51X,OPF9.3,10X,1PE11.4)
605  FORMAT(//35X,9HCENTER OF,9X,11HLOCATION OF,21X, 8HCOMPUTED/
135X,13HSLIT FUNCTION,5X,11HSLIT CENTER,5X,11HCALIBRATION,5X,
210HSLIT WIDTH/
335X, 9HANGSTROMS,9X,9HANGSTROMS,7X,6HFACTOR,10X,9HANGSTROMS//
435X,F9.3,9X,F9.3,6X,1PE11.4,4X,1PE11.4//)
606  FORMAT(//50X, 9HCENTER OF,12X, 8HCOMPUTED/
1      50X,13HSLIT FUNCTION,8X, 10HSLIT WIDTH/
2      50X, 9HANGSTROMS,12X,9HANGSTROMS//)
607  FORMAT(41X,45HSLIT FUNCTION SPECIFIED BY A GAUSSIAN PROFILE//)
608  FORMAT(31X,18HWAVELENGTH AT PEAK,8X, 4HPEAK,14X,18HWIDTH AT HALF-P
1EAK/31X,22HSENSITIVITY, ANGSTROMS,4X,11HSENSITIVITY,7X,
222HSENSITIVITY, ANGSTROMS//
339X,F9.3,11X,1PE11.4,12X,1PE11.4//)
609  FORMAT(50X,13HPEAK VALUE OF,5X,14HWIDTH AT HALF-/
1      50X,13HSLIT FUNCTION,5X,15HPEAK, ANGSTROMS//
2      52X,5H1.000,11X,1PE11.4)
610  FORMAT(//16X,96HSPECTRAL CALIBRATION OF INSTRUMENT THAT MULTIPLIES
1 SLIT FUNCTION TO YIELD INSTRUMENT SENSITIVITY//
250X,10HWAVELENGTH,11X,11HCALIBRATION/
350X, 9HANGSTROMS, 12X, 8HFUNCTION//)
612  FORMAT(////
1      51X,11HLOCATION OF,6X,17HINSTRUMENT OUTPUT/
2      51X,11HSLIT CENTER,6X,18H(W/CM2-MICRON-SR)*,/
3      51X, 9HANGSTROMS,8X, 19H(SENSITIVITY UNITS) //)
613  FORMAT(51X,OPF9.3,10X,1PE11.4,5A1)
615  FORMAT(33X,19HRADIOMETER OUTPUT ,1PE11.4,5A1,37H(W/CM2-MICRON-SR)
1*(SENSITIVITY UNITS)////)
616  FORMAT(//30X, 66H
1-----
2//)

C  FORMATS FOR ERROR STATEMENTS.

700  FORMAT(//26X,83HDETECTOR OMITTED BECAUSE PART OR ALL OF SENSITIVITY
1 LIES OUTSIDE COMPUTED SPECTRUM.//)
701  FORMAT(//26X,67HDETECTOR OMITTED BECAUSE WAVELENGTHS DO NOT INCREAS
1E MONOTONICALLY.//)
702  FORMAT(//5X,110HINPUT DATA FOR LAMS1 OR LAMS2 WOULD HAVE ALLOWED P
1ART OR ALL OF THE INSTRUMENT SENSITIVITY TO LIE OUTSIDE THE,/
24X, 96H COMPUTED SPECTRUM. THE END POINTS WERE APPROPRIATELY ADJUS
3TED SO THAT NOW THE SCANNING RANGE IS,/
44X, 5H FROM,F8.2,4H TO ,F8.2, 16H ANGSTROMS WITH , F6.3,
516H ANGSTROM STEPS.////)
703  FORMAT(10X,101HDETECTOR OMITTED BECAUSE WAVELENGTHS SPECIFYING SPE
1CTRAL CALIBRATION DO NOT BOUND DESIRED SCAN RANGE.//)
704  FORMAT(//8X,103HDETECTOR OMITTED BECAUSE SPECIFIED CENTER OF SLIT
1FUNCTION LIES OUTSIDE OF THE SPECIFIED SLIT FUNCTION.//)
705  FORMAT(// 17X,85HDETECTOR OMITTED BECAUSE UPPER SCAN LIMIT WAS INP
1UT LESS THAN OR EQUAL TO LOWER LIMIT//)

```

END

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$ORIGIN          ALPHA
$IBFTC HF075M

      SUBROUTINE GROWTH

C  SUBROUTINE GROWTH COMPUTES THE CURVE OF GROWTH.

      COMMON/CPL0T/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
      COMMON/CARRAY/ILAM(9000),ELAM( 9000)
      COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
      COMMON/CBAND1/ALPHAU,BEU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
1      ALPHAL,BEL,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL,TERML
      COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,MU,ALTNAT,
1      WEL,WEXEL,WEYEL,WEZEL,BVL,DVL,          NUSPIN
      COMMON/CTEMP/TELECT,TVIB,TROT
      COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
      COMMON/CTRAN/PARTCC,NUBARO,Q,AOE,CINT1,CINT2,KMIN,KMAX
      COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

      REAL LAM1,LAM2,LAMMAX,LAMMIN,ILAM,ILAM1,LAMBDA,LAMDA1,LAMDA2,
1      LAMDA3
      DIMENSION DEPTH(25),GROW(25)

      LAM1= READ1
      LAM2= READ2

C  PRINT HEADING FOR CURVE-OF-GROWTH CALCULATION.

      WRITE(6,600) LAM1,LAM2

C  IF THE UPPER WAVELENGTH LIMIT WAS INPUT FIRST, WRITE AN ERROR
C  MESSAGE AND OMIT THIS CURVE OF GROWTH.

      IF (LAM2 .LE. LAM1) GO TO 70

C  IF WAVELENGTH LIMITS ARE OUTSIDE SPECTRAL RANGE CONSIDERED, SET
C  INTEGRATION LIMITS TO APPROPRIATE END WAVELENGTH.

      IF (LAM1 .LT. LAMMIN) LAM1=LAMMIN
      IF (LAM2 .GT. LAMMAX) LAM2=LAMMAX

C  FIND INDICES IN INTENSITY ARRAY TO BE INCLUDED IN INTEGRATION.

      NSTART= 1.0 +(LAM1-LAMMIN)/DELLAM
      NEND= 1.0 +(LAM2-LAMMIN)/DELLAM

C  DEFINE SPECIAL WAVELENGTHS NEEDED IN THE INTEGRATION.

      COUNT= NSTART
      LAMDA1= LAMMIN+ (COUNT-1.0)*DELLAM
      LAMDA2= LAMDA1+ DELLAM
      COUNT= NEND
      LAMDA3= LAMMIN+ (COUNT-1.0)*DELLAM

C  INITIALIZE DEPTH AND START CURVE-OF-GROWTH CALCULATION.

      DEPTH= 3.162278E-7

      M2=NEND
      IF(NEND .NE. NARRAY) M2=NEND+1
      DO 60 M1=1,25
      TOTALI= 0.0
      DEPTH= DEPTH*3.162278
      DO 10 M=NSTART,M2
      IF (ELAM(M) .LE. 1.0E-36) GO TO 10
      COUNT=M
      LAMBDA=(LAMMIN + (COUNT-1.0)*DELLAM)*1.0E-8
      BLAM=1.1904E-16*EXP(-1.43879/(LAMBDA*TELECT))/(LAMBDA**5*
1      (1.0-EXP(-1.43879/(LAMBDA*TELECT))))
      CILAM1 =ALOG(8.40032E+15*LAMBDA**5*(1.0-EXP(-1.43879/
1      (LAMBDA*TELECT))))
      CILAM2=ALOG(DEPTH)
      CILAM3=ALOG(ELAM(M))
      CILAM4 =1.43879/(LAMBDA*TELECT)-2.30259*CINT3+CILAM1+CILAM2
1      +CILAM3
      IF (CILAM4 .GT. 87.0) CILAM4=87.0
      CILAM4=EXP(CILAM4)
      ILAM(M)=BLAM*(1.0-EXP(-CILAM4))
10      CONTINUE

C  TEST INTERVAL LIMITS.

      IF (NSTART .LT. NEND) GO TO 20

C  THE INTERVAL IS BOUNDED BY CONSECUTIVE ENTRIES IN THE LAMBDA ARRAY.

      SLOPE=(ILAM(NSTART+1)-ILAM(NSTART))/DELLAM
      TOTALI=((SLOPE*(LAM1-LAMDA1)+ILAM(NSTART))+(SLOPE*(LAM2-
1      LAMDA1)+ILAM(NSTART)))*(LAM2-LAM1)/2.0E+4
      GO TO 50

C  IS THERE A RIGHT-HAND INCREMENT.

20      IF (NEND.EQ.NARRAY) GO TO 30

C  COMPUTE INTEGRATED INTENSITY FROM RIGHT-HAND INCREMENTAL AREA.

```

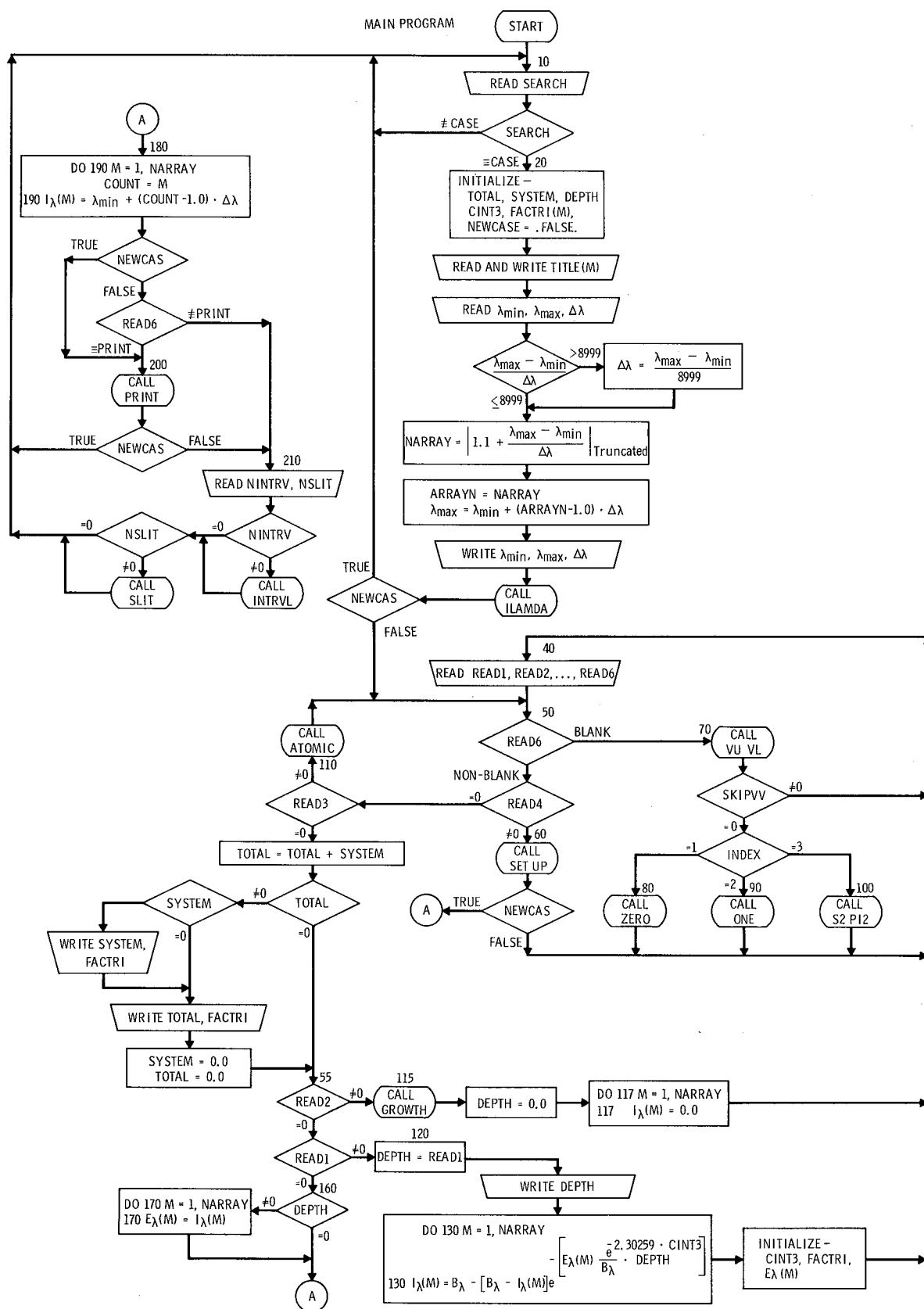
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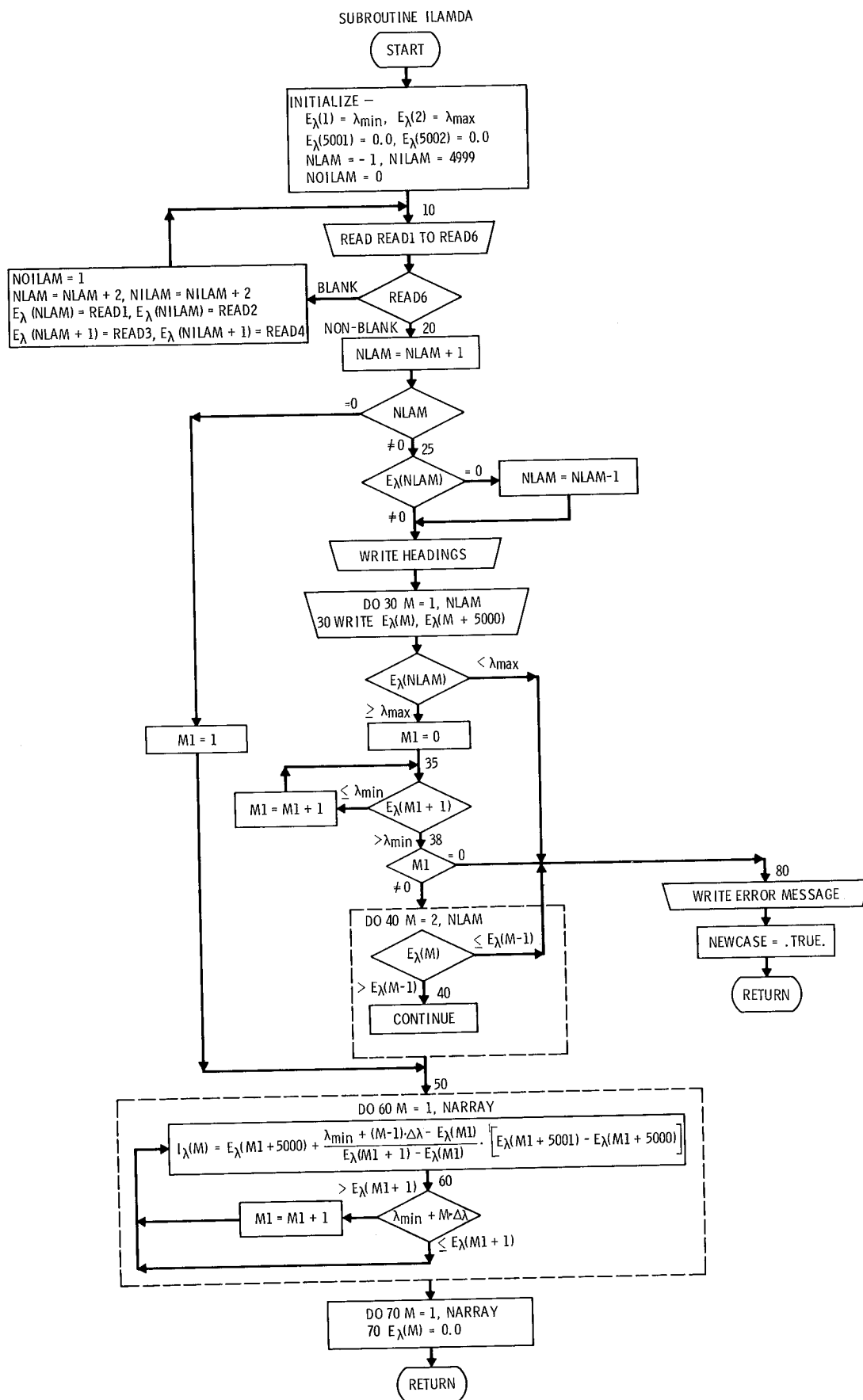
      ILAM1=(ILAM(NEND+1)-ILAM(NEND))*(LAM2-LAMDA3)/
1      DELLAM+ILAM(NEND)
      TOTALI=(ILAM1+ILAM(NEND))*(LAM2-LAMDA3)/2.0E+4
C  COMPUTE INTEGRATED INTENSITY FROM LEFT-HAND INCREMENTAL AREA.
30      ILAM1=(ILAM(NSTART)-ILAM(NSTART+1))*(LAMDA2-LAM1)/
1      DELLAM+ILAM(NSTART+1)
      TOTALI=TOTALI+(ILAM1+ILAM(NSTART+1))*(LAMDA2-LAM1)/2.0E+4
C  DO INTERVAL LIMITS BOUND A SINGLE ENTRY IN THE LAMBDA ARRAY.
      IF (NEND .EQ. NSTART+1) GO TO 50
C  COMPUTE INTEGRATED INTENSITY FROM CENTRAL INCREMENTAL AREAS.
      NSTART=NSTART+2
      DO 40 M=NSTART,NEND
40      TOTALI=TOTALI+(ILAM(M)+ILAM(M-1))*DELLAM/2.0E+4
C  RESET NSTART FOR NEXT STEP OF DO LOOP ENDING AT STATEMENT 60.
      NSTART=NSTART-2
50      DEPTH1(M1)= DEPTH
60      GROW(M1)= TOTALI
C  WRITE CURVE-OF-GROWTH DATA.
      WRITE(6,601) (DEPTH1(M),GROW(M), M=1,25)
      RETURN
C  THERE IS AN ERROR IN THE LIMITS FOR THE INTEGRATION INTERVAL.
70      WRITE(6,700) LAM1,LAM2
      RETURN
C  FORMATS FOR WRITE STATEMENTS.
600      FORMAT(//
1          34X,33H CURVE OF GROWTH CALCULATION FROM ,F8.2,4H TO ,F8.2,
2          10H ANGSTROMS//
3          70X,10H INTEGRATED/
4          52X, 9H GEOMETRIC,9X, 9H INTENSITY/
5          52X,9H DEPTH, CM,9X,12H WATTS/CM2-SR//)
601      FORMAT(52X,1PE9.3,10X,E9.3)
C  FORMAT FOR ERROR STATEMENT.
700      FORMAT(//10X,16H THE LOWER LIMIT ,1PE11.4,33H IS GREATER THAN THE U
1        PPER LIMIT ,E11.4,36H THUS INTEGRATION WAS NOT PERFORMED. )
      END
*****

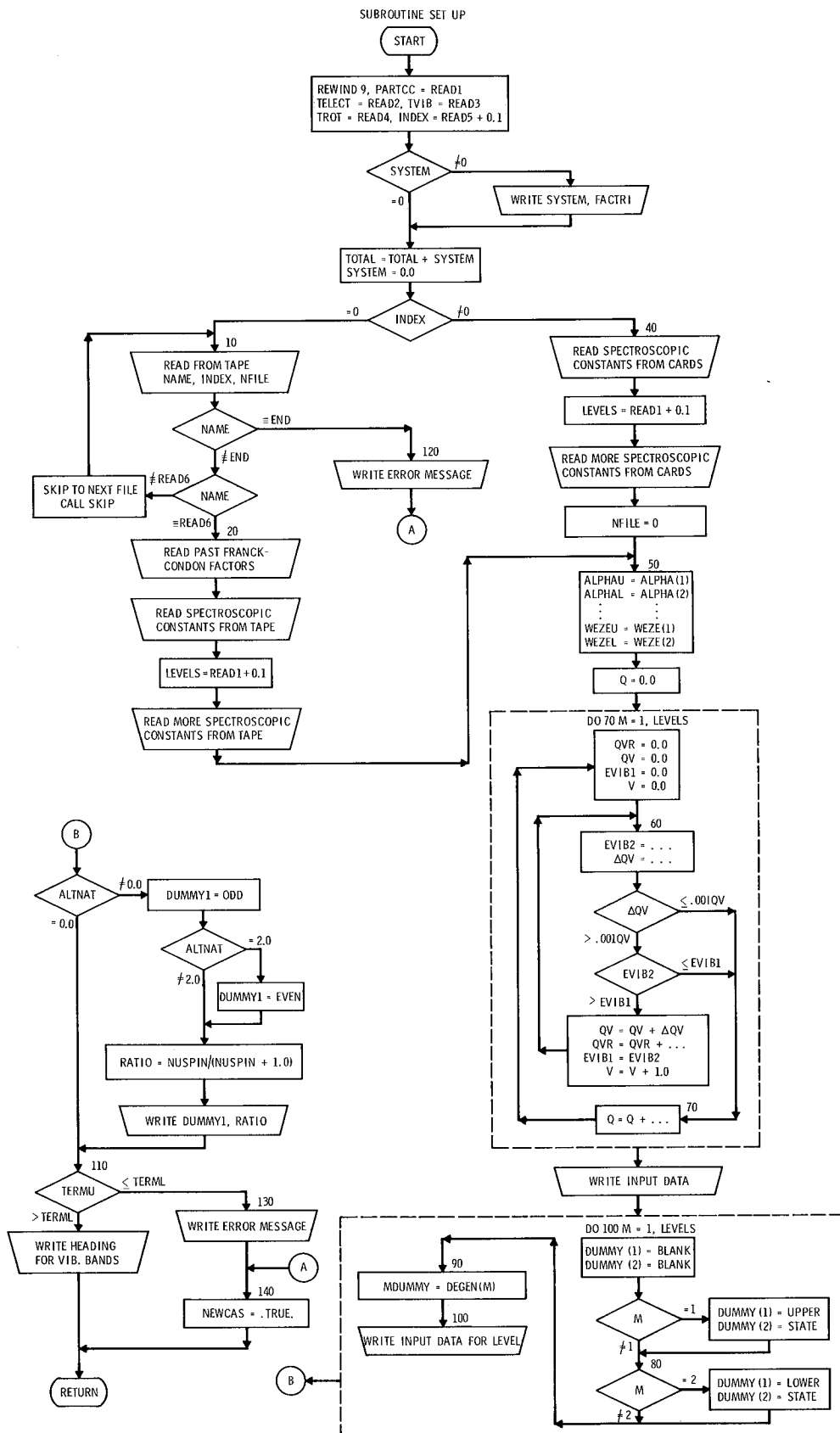
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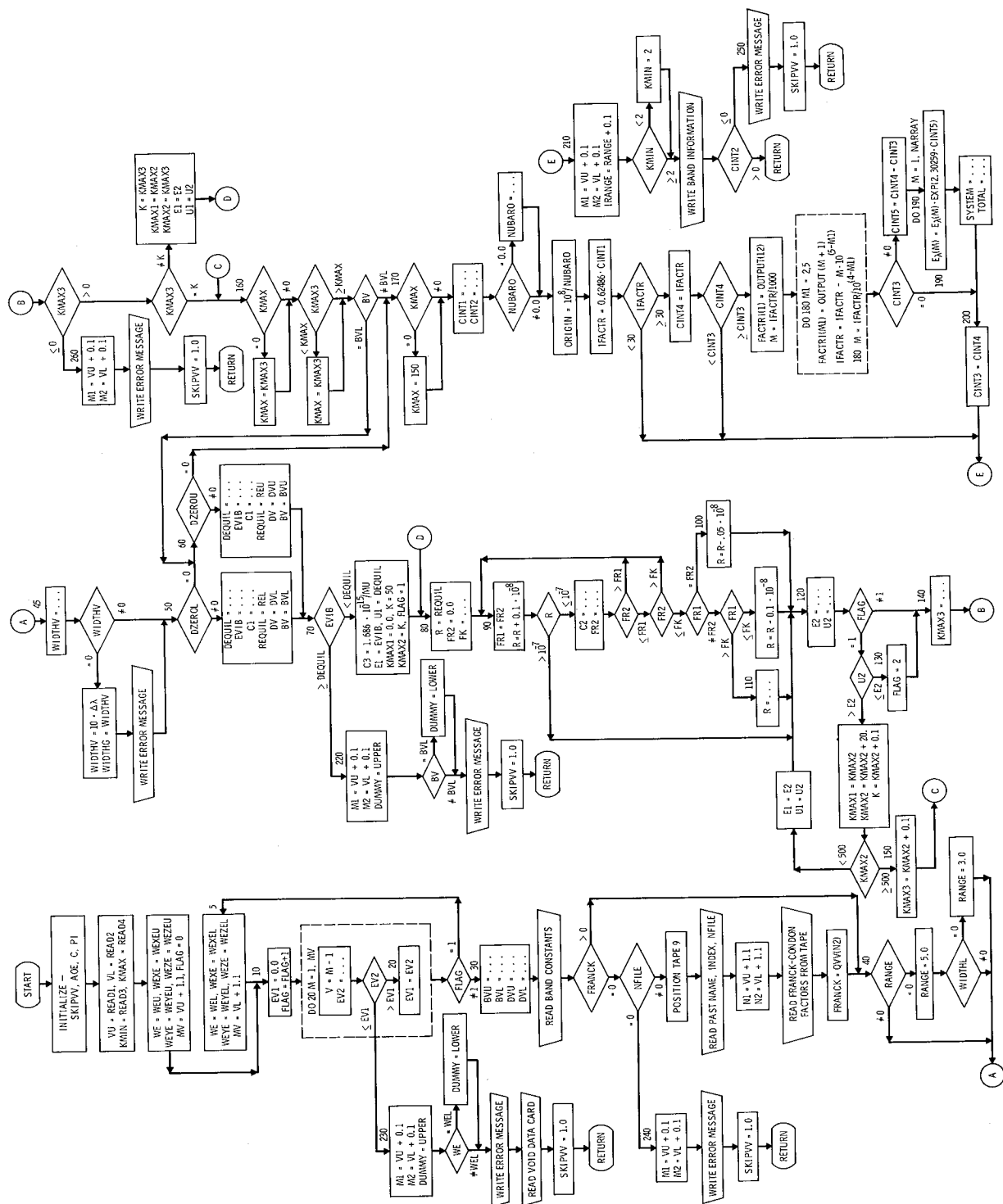
APPENDIX B

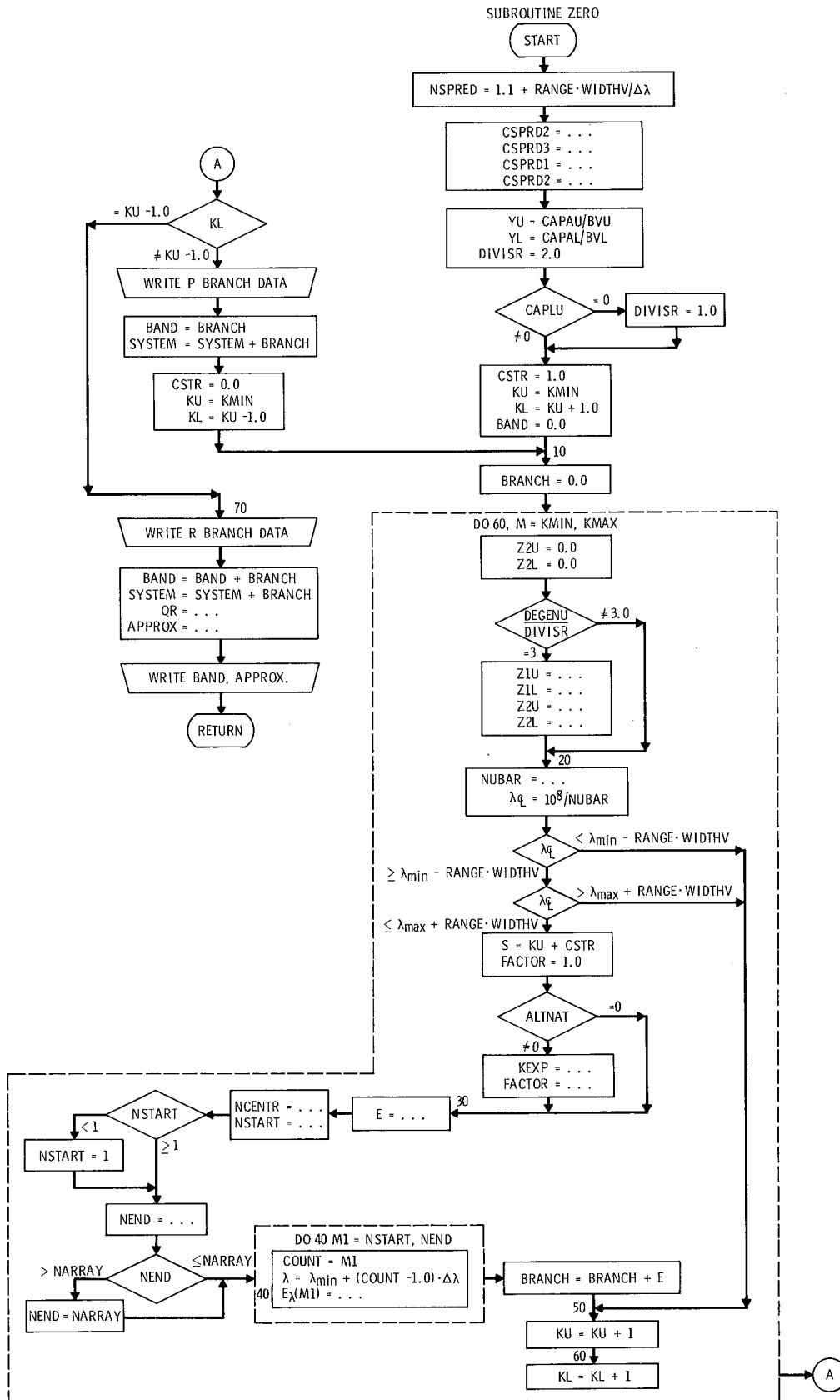
FLOW CHARTS OF PROGRAM



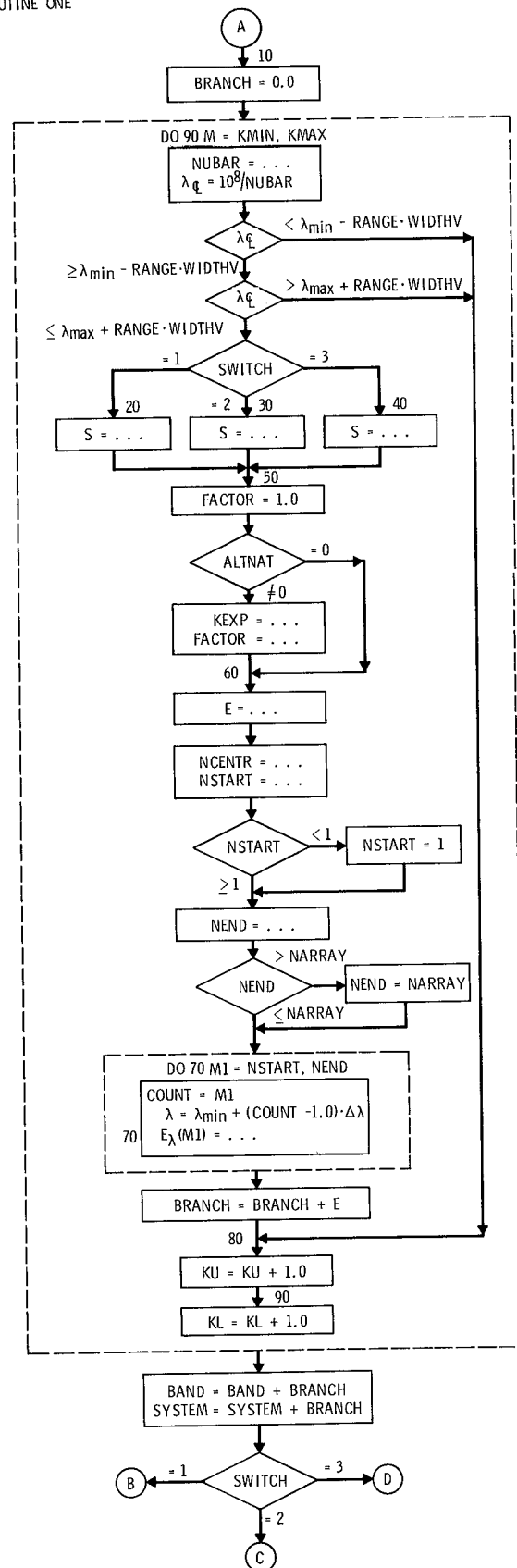
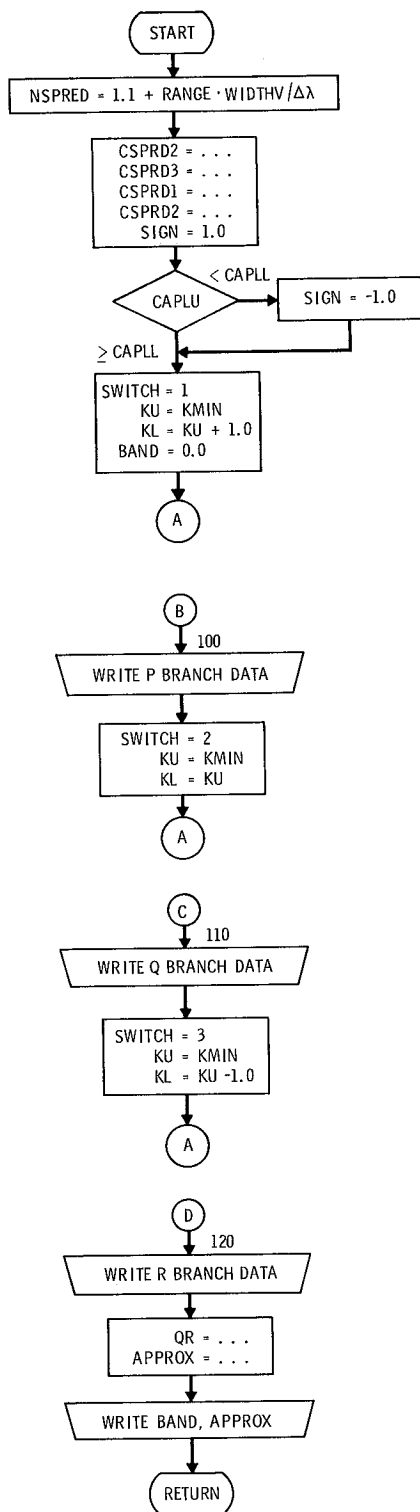


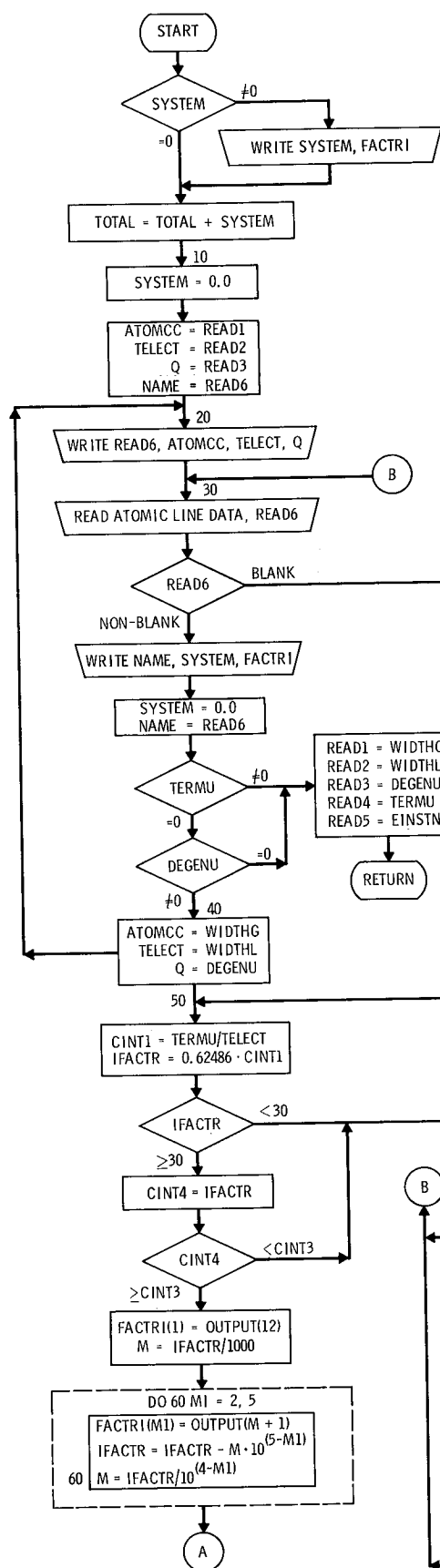




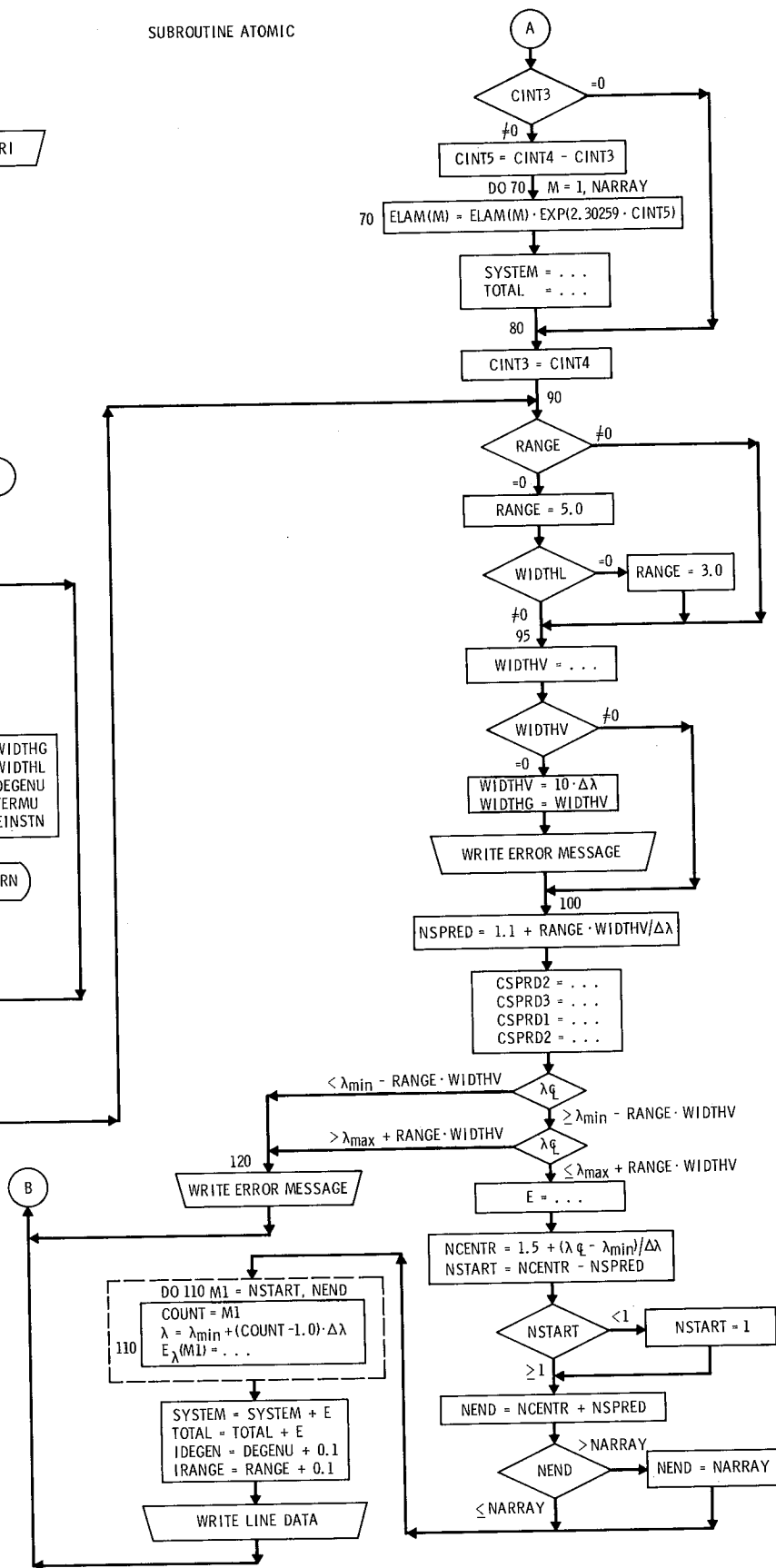


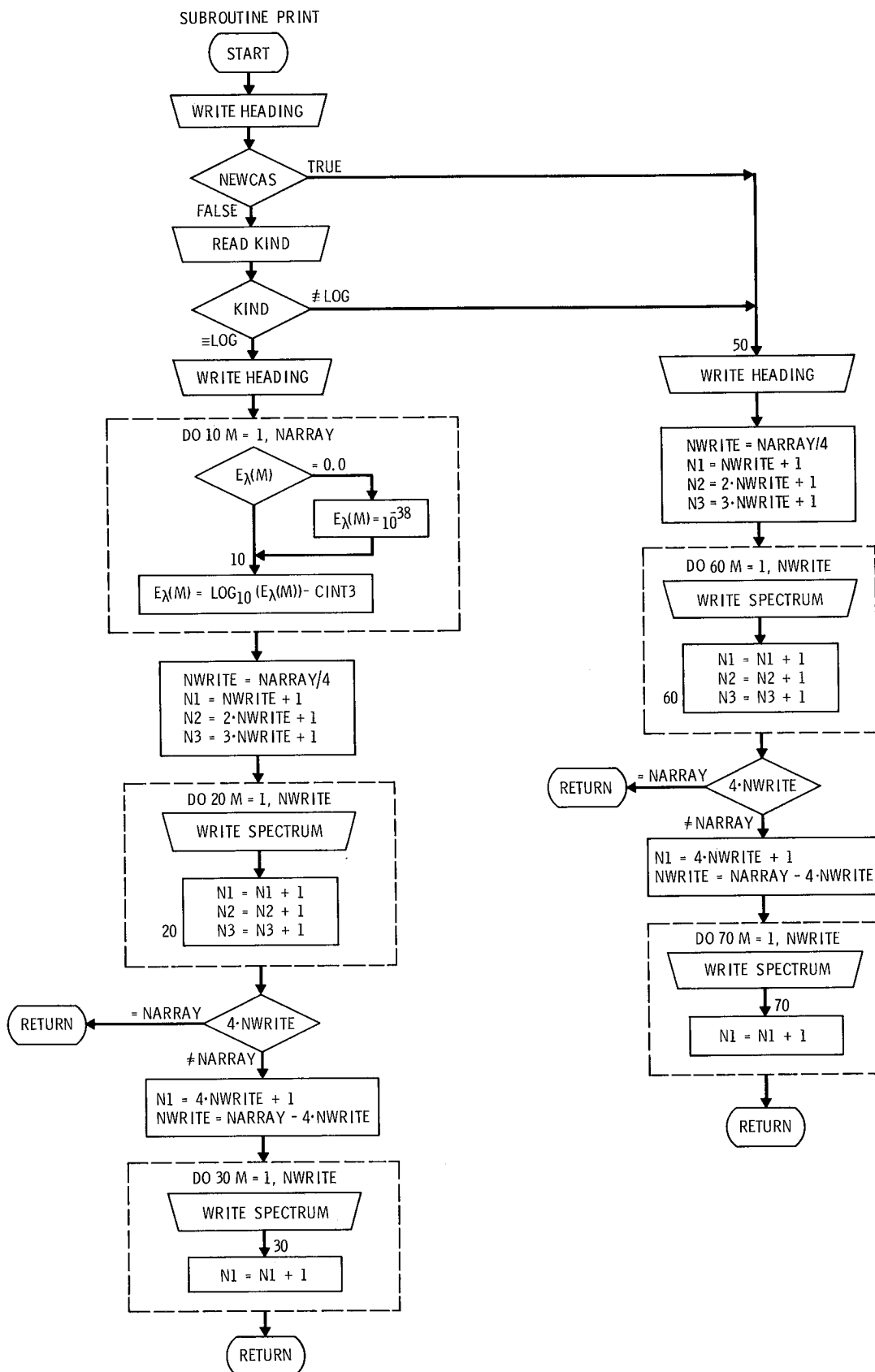
SUBROUTINE ONE

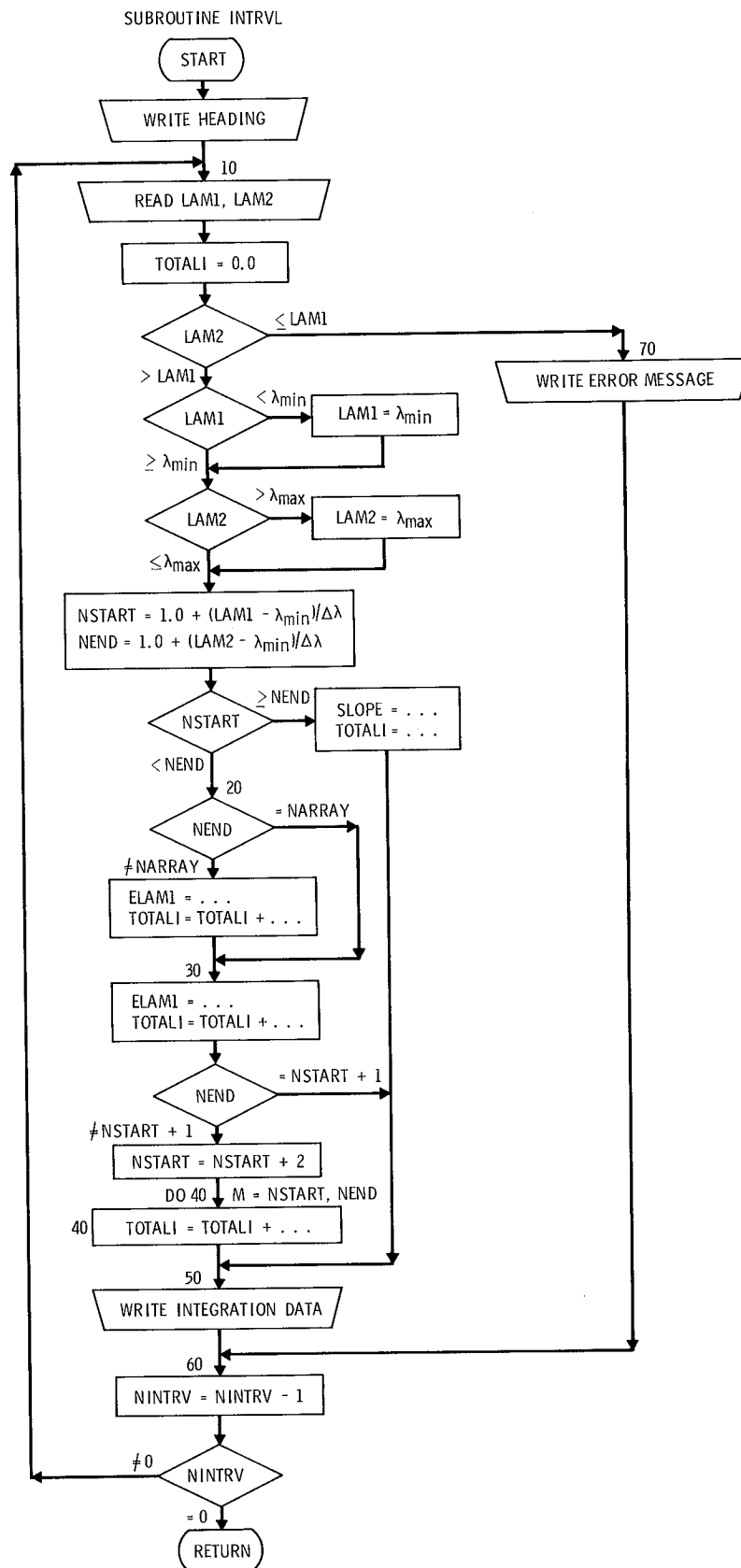




SUBROUTINE ATOMIC







APPENDIX C

DESCRIPTION OF INPUT CARDS FOR PROGRAM

Card number	Columns	Format	Content	Number of cards per case	Comments
Input required for each case					
1	1-4	A4	Case card CASE	1	Columns 1-4 must spell CASE. The remaining spaces may be used for data deck identification. This card is read in the main program.
2	1-72	12A6	Title card TITLES	3	Any 72 alphameric characters may be written in the first 72 spaces of each card. The information input on these cards will be written on the heading of each case. These cards are read in the main program.
3	1-10 11-20 21-30	E10.0 E10.0 E10.0	Spectral coverage and resolution IAMMIN, λ_{\min} IAMMAX, λ_{\max} DELLAM, $\Delta\lambda$	1	(IAMMAX-IAMMIN)/DELLAM \leq 8999. This card is read in the main program.
Incident spectrum cards, if specified					
4	1-10 11-20 21-30 31-40	E10.0 E10.0 E10.0 E10.0	Incident spectrum IAM(M), λ ILAM(M), I_{λ} LAM(M+1) ILAM(M+1)	0-2000	LAM(1) \leq IAMMIN, LAM(LAST) \geq IAMMAX. IAM(M) $<$ IAM(M+1) Blank cards are not required if an incident spectrum is not specified. Maximum number of points permitted is 4000. The last card can have only one point, if desired. If the final output is to be a curve of growth or an optically thin spectrum, an incident spectrum should not be specified. These cards are read in subroutine ILAMDA.

Card number	Columns	Format	Content	Number of cards per band system	Comments
BAND SYSTEM CARDS: Two alternatives - Band system can be input from magnetic tape or from cards. Band systems input from magnetic tape					
5			Band system data and name	1	Any number of band systems can be included in a layer or a case.
	1-10	E10.0	PARTCC, N		
	11-20	E10.0	TELECT, Telect		Name must be left justified and must be exactly one of the following:
	21-30	E10.0	TVIB, Tvib		
	31-40	E10.0	TROT, Trot		
	67-72	A6	NAME		
					CNbVbb CNbRED CØb4+b CH4300
					C2SWAN ØH3060 N2+b1- BEXB-X
					CØASDI C2PHIL N2b1+b NØbBbb
					CØ+bCT Ø2bSRb N2b2+b NØbGbb
					N2LBH CH3900
					b \equiv blank space. This card is read in the main program, subroutine ILAMDA, or subroutine ATOMIC.
Band system input from cards					
5-a			Band system data and name	1	Any number of band systems can be included in a layer or a case.
	1-10	E10.0	PARTCC, N		
	11-20	E10.0	TELECT, Telect		
	21-30	E10.0	TVIB, Tvib		Name can be any A6 identifier.
	31-40	E10.0	TROT, Trot		
	41-45	F5.0	INDEX		IF CAPLU - CAPLL = 0 INDEX = 1.0
	67-72	A6	NAME		If CAPLU - CAPLL = ± 1 and this is not a $2\pi \leftrightarrow 2\pi$ (or vice versa) transition
					INDEX = 2.0. If this is a $2\pi \leftrightarrow 2\pi$ (or vice versa) transition INDEX = 3.0.
					This card is read in the main program, subroutine ILAMDA, or subroutine ATOMIC.

Card number	Columns	Format	Content	Number of cards per band system	Comments
5-b			Band system data	1	This card is read in subroutine SETUP.
	1-10	E10.0	LEVELS		
	11-20	E10.0	ALTNAT, C		
	21-30	E10.0	DEU, D _e '		
	31-40	E10.0	BETAU, β_e		
	41-50	E10.0	REU, r _e '		
	51-60	E10.0	DZEROU, D _O '		
	61-70	E10.0	CAPAU, A'		
	71-80	E10.0	CAPLU, Λ'		
5-c			Band system data	1	This card is read in subroutine SETUP.
	1-10	E10.0	MU, μ_A		
	11-20	E10.0	NUSPIN, I		
	21-30	E10.0	DEL, D _e "		
	31-40	E10.0	BETAL, β_e		
	41-50	E10.0	REL, r _e "		
	51-60	E10.0	DZEROL, D _O "		
	61-70	E10.0	CAPAL, A"		
	71-80	E10.0	CAPLL, Λ "		
5-d			Spectroscopic constants	LEVELS	The appropriate cards for the upper and lower levels of the transition must be input first and second, respectively. These cards are read in subroutine SETUP.
	1-10	E10.0	DEGEN(M), d		
	11-20	E10.0	TERM(M), T _e		
	21-30	E10.0	WE(M), ω_e		
	31-40	E10.0	WEXE(M), $\omega_e x_e$		
	41-50	E10.0	WEYE(M), $\omega_e y_e$		
	51-60	E10.0	WEZE(M), $\omega_e z_e$		
	61-70	E10.0	BE(M), B _e		
	71-80	E10.0	ALPHA(M), α_e		

Card number	Columns	Format	Content	Number of cards per band system	Comments
Vibrational band cards for each system					
6			VU-VL data	Any number	Cards 6 and 7 specify one vibrational band. Any number of bands may be input and these must follow card number 5 if the band system is input from tape, or 5-d if the input is from cards. KMIN and KMAX may be left blank. If KMIN is left blank, it will be set to 2. If KMAX is left blank and a value for DZEROU and/or DZEROL is known, KMAX will be computed; otherwise KMAX will be set to 150. This card is read in the main program.
	1-10	E10.0	VU, v'	but each	
	11-20	E10.0	VL, v''	must be	
	21-30	E10.0	KMIN, K _{min}	followed by	
	31-40	E10.0	KMAX, K _{max}	a card 7.	
7			VU-VL data	Any number	NUBARO and RANGE may be left blank. If NUBARO is left blank, its value will be computed from the spectroscopic constants. If RANGE is left blank, it will be set to 5 if WIDTHL \neq 0; if WIDTHL = 0, RANGE will be set to 3. FRANCK may be left blank for a band system input from tape. If this is done, the value stored on tape is used in the calculation. This card is read in subroutine VU VL.
	1-10	E10.0	SUMRE2, $\Sigma \left \frac{\text{Re}(\bar{v}'v'')}{ea_0} \right ^2$		
	11-20	E10.0	WIDTHG, w _g		
	21-30	E10.0	WIDTHL, w _l		
	31-40	E10.0	NUBARO, $\bar{v}_0(v'v'')$		
	41-50	E10 0	FRANCK, q _{v'v''}		
	51-60	E10 0	RANGE		

Card number	Columns	Format	Content	Number of cards per atomic system	Comments
Atomic system input cards					
8			Atomic data	1	NAME can be any A6 identifier. Any number of atomic systems can be specified for each layer and they can be mixed with the specified band systems. However, the printed output will be easier to read if all the atomic systems are either input before or after the band systems. This card is read either in the main program, subroutine ILAMDA, or ATOMIC.
	1-10	E10.0	ATOMCC, N		
	11-20	E10.0	TELECT, T _{elect}		
	21-30	E10.0	Q, Q		
	67-72	A6	NAME		
9			Atomic data	Any number following each card 8	RANGE may be left blank. If this is done and WIDTHL \neq 0, RANGE is set to 5; otherwise, RANGE is set to 3. This card is read in subroutine ATOMIC.
	1-10	E10.0	WIDTHG, W _g		
	11-20	E10.0	WIDTHL, W _l		
	21-30	E10.0	DEGENU, d'		
	31-40	E10.0	TERMU, T' _e		
	41-50	E10.0	EINSTN, A _{ul}		
	51-60	E10.0	LAMCL, λ_{cl}		
	61-66	E6.0	RANGE		

Card number	Columns	Format	Content	Number of cards per case	Comments
Curve-of-growth card					
10			Curve-of-growth integration limits IAML, λ IAM2, λ GROWTH	Any number.	<p>IAML < IAM2, IAML \geq IAMMIN, IAM2 \leq IAMMAX</p> <p>This card specifies that a curve-of-growth will be printed on the output sheet. The card must follow the last vibrational band or atomic line card. Any number of integration intervals IAML to IAM2 may be specified, and the word GROWTH must appear on each card. Blank cards are not required if a curve of growth is not needed. A curve-of-growth calculation can be specified for any single-layer case or for the first layer of a multilayer case. However, if an incident spectrum is specified, it will not be used and, in fact, will be re-initialized to zero. This card is read in the main program or subroutine ATOMIC.</p>
Radiative transport card					
11			Depth of radiating layer DEPTH, l , x LAYER	One for each layer.	<p>LAYER must be left-justified. If the "true" spectrum for a given incident spectrum and geometric DEPTH is to be computed, this card must be input with the word LAYER written as indicated. This card follows the last curve-of-growth card. If a "true" spectrum is not to be computed, and the final output is to be for an optically thin spectrum, this card is omitted. This card is read in the main program or subroutine ATOMIC.</p>

Card number	Columns	Format	Content	Number of cards per case	Comments
Print spectrum cards					
12	67-72	A6	Specification of whether or not spectrum is to be printed. OUTPUT	1	OUTPUT must be left-justified. 1. To print the spectrum, OUTPUT = PRINT. 2. To not print the spectrum, OUTPUT = NONE. This card is read in subroutine ATOMIC or the main program. KIND must be left-justified.
13	67-72	A6	Specification of type of printed output KIND	0 or 1	1. If it is desired to print \log_{10} (intensity), KIND = LOG 2. If it is desired to print intensity directly, KIND is left blank. This card is required only if a printed spectrum was specified on card 12. This card is read in subroutine PRINT.
Number of intervals and slits card					
14	1-5 6-10	I5 I5	Specification of number of intervals and slits NINTRV NSLIT	1	If no intervals or slits are desired, a blank card must be included, and it will be the last card in the case. This card is read in the main program.
Interval cards					
15	1-10 11-20	E10.0 E10.0	Integration limits for interval. LAM1, λ LAM2, λ	NINTRV	LAM1 < LAM2 LAM1 \geq LAMMIN, LAM2 \leq LAMMAX These cards must follow card 14. These cards are read in subroutine INTRVL.

Card number	Columns	Format	Content	Number of cards per slit case	Comments
Slit cards: There are four types of slits and any number of each may be specified for each case. The total number of SLITS must be equal to NSLIT. The slit types are: (a) fixed Gaussian, (b) fixed linear, (c) scanning Gaussian, and (d) scanning linear.					
(a) Fixed Gaussian slit cards					
16-a	1-4	A4	Slit identification SLIT	1	The first four columns of this card must spell SLIT. The remaining columns can contain any desired information. This card is read in subroutine SLIT.
17-a	1-5	I5	NPOINT	1	NPOINT = 0 (or blank) for this slit case. This card is read in subroutine SLIT.
18-a	1-10 11-20 21-30	E10.0 E10.0 E10.0	Slit data IAMCL RIAMCL WIDTH	1	IAMCL \pm 3.0(WIDTH) must fall between IAMMAX and IAMMIN. IAMCL = spectral location of slit center. RIAMCL = peak value of instrument sensitivity. WIDTH = width of slit at half-peak sensitivity. This card is read in subroutine SLIT.
(b) Fixed linear slit cards					
16-b	1-4	A4	Slit identification SLIT	1	The first four columns of this card must spell SLIT. The remaining columns can contain any desired information. This card is read in subroutine SLIT.
17-b	1-5 25-34	I5 E10.0	NPOINT IAMS1	1	NPOINT \leq 100 and IAMS1 must not allow any part of the instrument sensitivity to fall outside the computed spectrum. ¹ This card is read in subroutine SLIT.

¹IAMS1 = spectral location at which slit function will be centered.

Card number	Columns	Format	Content	Number of cards per slit case	Comments
18-b	1-10 11-20 21-30 31-40 41-50 51-60	E10.0 E10.0 E10.0 E10.0 E10.0 E10.0	Slit function LAM(M) RSLIT(M) LAM(M + 1) RSLIT(M + 1) LAM(M + 2) RSLIT(M + 2)	Enough to specify NPOINT pairs of slit function data points.	The slit function abscissa must be in Å, but they can be relative to any origin desired. IAM(M) < IAM(M + 1) These cards are read in subroutine SLIT.
19-b	1-10 11-20	E10.0 E10.0	Slit function data LAMCL RIAMCL	1	LAMCL = position in slit function to be located at LAMS1. RIAMCL = calibration factor. The instrument sensitivity is given by the product RIAMCL • RSLIT(M). IAM(1) ≤ IAMCL ≤ LAM(NPOINT) This card is read in subroutine SLIT.
(c) Scanning Gaussian slit cards					
16-c	1-4	A4	Slit identification SLIT	1	The first four columns of this card must spell SLIT. The remaining columns can contain any desired information. This card is read in subroutine SLIT.
17-c	1-5 10 15-24 25-34 35-44 46-50	I5 I1 E10.0 E10.0 E10.0 I5	Slit data NPOINT SCAN STEP LAMS1 LAMS2 NRLAMS	1	NPOINT = 0, SCAN = 1, STEP = distance between steps in SCAN, LAMS1 = starting wavelength of SCAN, LAMS2 = stopping wavelength of SCAN, NRLAMS = number of pairs of values specifying the spectral calibration of the instrument. LAMS1 ≥ LAMMIN + 3.0(WIDTH) LAMS2 ≤ LAMMAX - 3.0(WIDTH) This card is read in subroutine SLIT.
18-c	21-30	E10.0	WIDTH	1	WIDTH = width of slit function at half-peak height. This card is read in subroutine SLIT.

Card number	Columns	Format	Content	Number of cards per slit case	Comments
19-c	1-10 11-20 21-30 31-40 41-50 51-60	E10.0 E10.0 E10.0 E10.0 E10.0 E10.0	Spectral calibration IAMR(M) RIAM(M) IAMR(M + 1) RIAM(M + 1) IAMR(M + 2) RIAM(M + 2)	Enough to specify NRLAMS pairs of spectral calibration points	The instrument sensitivity at any wavelength along the scan is given by the spectral calibration at the slit function center. Interpolated values of the spectral calibration are used when appropriate. IAMR(M) < IAMR(M + 1) IAMR(1) ≤ IAMS1, IAMR(NRLAMS) ≥ IAMS2.
(d) Scanning linear slit cards					
16-d	1-4	A4	Slit identification SLIT	1	The first four columns of this card must spell SLIT. The remaining columns can contain any desired information. This card is read in subroutine SLIT.
17-d	1-5 10 15-24 25-34 35-44 46-50	I5 I1 E10.0 E10.0 E10.0 I5	Slit data NPOINT SCAN STEP IAMS1 IAMS2 NRLAMS	1	NPOINT ≤ 100. All other comments made for card 17-c of the scanning Gaussian slit apply here as well. This card is read in subroutine SLIT.
18-d	1-10 11-20 21-30 31-40 41-50 51-60	E10.0 E10.0 E10.0 E10.0 E10.0 E10.0	Slit function IAM(M) RSLIT(M) IAM(M + 1) RSLIT(M + 1) IAM(M + 2) RSLIT(M + 2)	Enough to specify NPOINT pairs of slit function data points	The slit function abscissa must be in Å but they can be relative to any origin desired. IAM(M) < IAM(M + 1) These cards are read in subroutine SLIT.

Card number	Columns	Format	Content	Number of cards per slit case	Comments
19-d	1-10	E10.0	Slit function data LAMCL	1	LAMCL = position in the slit function that locates the slit during each step of the scan. $LAM(1) \leq LAMCL \leq LAM(NPOINT)$ This card is read in subroutine SLIT.
20-d	1-10 11-20 21-30 31-40 41-50 51-60	E10.0 E10.0 E10.0 E10.0 E10.0 E10.0	Spectral calibration LAMR(M) RIAM(M) LAMR(M + 1) RIAM(M + 1) LAMR(M + 2) RIAM(M + 2)	Enough to specify NRIAMS pairs of spectral calibration points	Comments for card number 19-c in the scanning Gaussian case apply here as well.

APPENDIX D

LISTING OF SPECTROSCOPIC CONSTANTS AND FRANCK-CONDON FACTORS FOR MOLECULAR BAND SYSTEMS ON MAGNETIC TAPE

In the listing of the Franck-Condon factors, values of 0.0 are printed as a row of stars (*).

DIATOMIC INDEX NO. NUMBER
TRANSITION SPECIFYING SPECIFYING
CN V SUBROUTINE DATA LOCATION
1 USED IN CALC. CN TAPE
1

SPECTROGRAPHIC CONSTANTS FOR A AND X STATES FROM POLETTI AND RIGUTTI,
NAOVO CIMENTO 39, P515, (1965).
E STATE DATA FROM HERZBERG EXCEPT WE AND WEKE WHICH WERE TAKEN FROM
DOUGLAS AND ROULTY ASTROPHYS J. SUPP.1, P295 (1954)
RKR FRANCK-CONDON FACTORS FROM SPINDLER JQSRT VOL. 5, P 165 (1965).
DISSOCIATION ENERGIES BASED ON HERZBERG P.455 AND ADJUSTED TO 8.2 EV.
THIS TRANSITION COMPUTED IN SUBROUTINE ZERO.

LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT	SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
C.	C.O	3	6.4643						
UPPER STATE	0.00	C		0.0000000E-38	0.0000000E-38	0.5950000E 05	C.1149300E-07		
LOWER STATE	0.00	C		0.0000000E-38	0.0000000E-38	0.6620000E 05	0.1171900E-07		

	ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEKE	WEYE	WEZE	BE	ALPHA E
UPPER STATE	2	2.5751800E 04	2.1686140E 03	2.0200000E 01	0.0000000E-39	0.0000000E-39	1.9701000E 00	2.2150000E-02
LOWER STATE	2	0.0000000E-39	2.0687450E 03	1.3134000E 01	-5.5000000E-03	0.0000000E-39	1.8992000E 00	1.7013300E-02
	4	9.2453440E 03	1.8125550E 03	1.2608600E 01	-1.1800000E-02	0.0000000E-39	1.7151000E 00	1.7075700E-02

FRANCK-CONDON FACTOR

VV	0	1	2	3	4	5	6	7	8	9
0	5.1790E-01	7.6000E-02	5.8000E-03	3.0000E-04	*****	*****	*****	*****	*****	*****
1	8.0900E-02	7.7950E-01	1.2400E-01	1.4300E-02	1.2000E-03	1.0000E-04	*****	*****	*****	*****
2	1.2000E-03	1.4170E-01	6.7540E-01	1.5500E-01	2.3900E-02	2.6000E-03	2.0000E-04	*****	*****	*****
3	*****	2.8000E-03	1.9050E-01	5.5290E-01	1.7450E-01	3.4200E-02	4.6000E-03	5.0000E-04	1.0000E-04	*****
4	*****	*****	4.3000E-03	2.3180E-01	5.2790E-01	1.8250E-01	4.5200E-02	7.1000E-03	1.0000E-03	1.0000E-04
5	*****	*****	1.0000E-04	5.4000E-03	2.6680E-01	4.8240E-01	1.7810E-01	5.5400E-02	9.7000E-03	1.7000E-03
6	*****	*****	*****	2.0000E-04	5.0000E-03	2.9330E-01	4.5830E-01	1.6400E-01	6.3900E-02	1.2300E-02
7	*****	*****	*****	*****	7.0000E-04	3.2000E-03	3.0950E-01	4.5540E-01	1.4250E-01	7.0800E-02
8	*****	*****	*****	*****	1.7000E-03	9.0000E-04	3.1220E-01	4.7500E-01	1.1460E-01	5.1840E-01
9	*****	*****	*****	*****	3.1000E-03	1.0000E-04	1.0000E-04	2.5560E-01	5.1840E-01	5.1840E-01
10	*****	*****	*****	*****	*****	*****	5.0000E-03	5.0000E-03	2.5370E-01	2.5370E-01
11	*****	*****	*****	*****	*****	*****	*****	6.7000E-03	2.0400E-02	2.0400E-02
12	*****	*****	*****	*****	*****	*****	*****	3.0000E-04	6.4000E-03	6.4000E-03
13	*****	*****	*****	*****	*****	*****	*****	1.0000E-04	1.4000E-03	1.4000E-03
14	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
15	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
16	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
17	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
18	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
19	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

VV	10	11	12	13	14	15	16	17	18	19
0	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
2	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
3	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
4	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
5	3.0000E-04	*****	*****	*****	*****	*****	*****	*****	*****	*****
6	2.4000E-03	4.0000E-04	1.0000E-04	*****	*****	*****	*****	*****	*****	*****
7	1.4100E-02	3.1000E-03	5.0000E-04	1.0000E-04	*****	*****	*****	*****	*****	*****
8	7.6600E-02	1.4800E-02	3.7000E-03	7.0000E-04	1.0000E-04	*****	*****	*****	*****	*****
9	8.1500E-02	8.2800E-02	1.3500E-02	4.1000E-03	7.0000E-04	1.0000E-04	*****	*****	*****	*****
10	5.8010E-01	4.9500E-02	9.0100E-02	1.1100E-02	4.6000E-03	7.0000E-04	1.0000E-04	*****	*****	*****
11	1.6970E-01	6.4470E-01	2.2700E-02	1.0240E-01	7.9000E-03	5.1000E-03	7.0000E-04	2.0000E-04	*****	*****
12	4.8100E-02	1.1310E-01	6.9670E-01	4.5000E-03	1.1950E-01	4.2000E-03	6.0000E-03	5.0000E-04	2.0000E-04	*****
13	3.7000E-03	8.5400E-02	4.2900E-02	7.1270E-01	1.0000E-04	1.4430E-01	9.0000E-04	7.8000E-03	3.0000E-04	*****
14	3.4000E-03	4.0000E-04	1.2030E-01	2.6600E-03	6.7620E-01	7.5000E-03	1.7790E-01	2.0000E-04	1.1000E-02	*****
15	*****	5.5000E-03	2.2000E-03	1.3800E-01	1.6000E-02	5.7860E-01	2.1100E-02	2.1670E-01	4.8000E-03	*****
16	1.0000E-04	5.0000E-04	5.6000E-03	1.6000E-02	1.2340E-01	9.1800E-02	4.3190E-01	3.2000E-02	2.5450E-01	*****
17	*****	*****	2.0000E-03	2.0000E-02	4.4700E-02	7.7000E-02	2.1000E-01	2.6890E-01	3.1300E-02	*****
18	*****	*****	*****	4.0000E-03	1.0000E-04	7.9000E-02	2.2900E-02	3.2340E-01	1.2800E-01	*****
19	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

DIATOMIC
TRANSITION
CN REC

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
3

NUMBER
SPECIFYING
DATA LOCATION
ON TAPE
2

SPECTROGRAPHIC CONSTANTS FOR A AND X STATES FROM POLETTI AND RIGUTTI,
NACVO CIMENTO 39, P 519, (1965).
B STATE DATA FROM HERZBERG EXCEPT WE AND WEKE WHICH WERE TAKEN FROM
DOUGLAS AND RUTLY ASTROPHYS J. SUPP.1, P 295 (1954)
SPIN COUPLING CONSTANT A TAKEN FROM HERZBERG WHICH IS CLOSE TO
AVERAGE VALUE BY POLETTI AND RIGUTTI'S
THIS TRANSITION COMPUTED IN SUBROUTINE S2 P12

LINE
ALTERNATION
FACTOR

NUCLEAR SPIN
FOR HOMONUCLEAR
MOLECULES

NUMBER OF
ELECTRONIC
LEVELS

REDUCED
ATOMIC
WEIGHT

0.

0.0

3

6.4643

SPIN
COUPLING
CONSTANT

QUANTUM NUMBER CF
RESULTANT ELECTRONIC ANGULAR
MOMENTUM ABOUT INTERNUC. AXIS

ROTATIONAL
CONSTANT
DE, 1/CM

ROTATIONAL
CONSTANT
BETA, 1/CM

DISSOCIATION
ENERGY
DEZERO, 1/CM

INTERNUCLEAR DISTANCE
AT EQUILIBRIUM
POSITION, CM

UPPER STATE -52.2C 1 0.5932700E-05 -0.4246000E-07 0.5740000E 05 0.1233200E-C7

LOWER STATE 0.00 0 0.6392000E-05 -0.9570000E-08 0.6620000E 05 0.1171900E-07

ELECTRONIC
DEGENERACY

ELECTRONIC
TERM ENERGY

WE

WEKE

WEYE

WEZE

BE

ALPHA E

UPPER STATE 4 9.2453440E 03 1.8125550E 03 1.2608600E 01 -1.1800000E-02 0.0000000E-39 1.7151000E 00 1.7075700E-02

LOWER STATE 2 0.0000000E-39 2.0687450E 03 1.3134000E 01 -5.5000000E-03 0.0000000E-39 1.8992000E 00 1.7013300E-02

2 2.5751800E 04 2.1686140E 03 2.0200000E 01 0.0000000E-39 0.0000000E-39 1.9701000E 00 2.2150000E-02

FRANCK-CONDON FACTOR

VV	C	1	2	3	4	5	6	7	8	9
V										
0	5.0015E-01	3.7105E-01	1.1065E-01	1.6700E-02	1.4000E-03	1.0000E-04	*****	*****	*****	*****
1	3.1785E-01	4.6000E-02	3.5275E-01	2.2335E-01	5.3550E-02	6.1500E-03	4.0000E-04	*****	*****	*****
2	1.2685E-01	2.4085E-01	1.1600E-02	2.1355E-01	2.8715E-01	1.0265E-01	1.5900E-02	1.2500E-03	5.0000E-05	*****
3	4.0200E-02	1.9420E-01	9.9500E-02	8.7800E-02	8.7850E-02	2.9940E-01	1.5665E-01	3.1300E-02	2.9500E-03	1.0000E-04
4	1.1100E-02	9.4100E-02	1.8115E-01	1.6150E-02	1.4890E-01	1.5950E-02	2.6685E-01	2.0665E-01	5.2850E-02	6.0000E-03
5	2.8500E-03	3.6150E-02	1.3300E-01	1.2280E-01	1.8000E-03	1.5905E-01	7.5000E-04	2.0690E-01	2.4545E-01	7.9800E-02
6	7.5000E-04	1.2200E-02	6.7550E-02	1.4155E-01	5.8700E-02	3.0400E-02	1.2870E-01	2.4000E-02	1.3895E-01	2.6755E-01
7	2.0000E-04	3.8000E-03	2.8100E-02	9.5000E-02	1.2095E-01	1.5050E-02	6.9600E-02	8.0950E-02	6.3450E-02	7.7700E-02
8	5.0000E-05	1.1000E-03	1.0400E-02	4.8550E-02	1.0880E-01	8.4400E-02	1.5000E-04	9.7700E-02	3.6500E-02	1.0080E-01
9	*****	3.5000E-04	3.6000E-03	2.1250E-02	6.8550E-02	1.0680E-01	4.5550E-02	9.4500E-03	1.0500E-01	8.2500E-03
10	*****	1.0000E-04	1.1500E-03	8.4500E-03	3.5300E-02	8.3050E-02	9.0100E-02	1.6100E-02	3.1900E-02	9.2500E-02
11	*****	*****	3.5000E-04	3.1500E-03	1.6000E-02	5.0200E-02	8.8800E-02	6.5150E-02	1.6500E-03	5.5850E-02
12	*****	*****	1.5000E-04	1.1000E-03	6.6500E-03	2.5900E-02	6.3150E-02	8.4400E-02	3.8350E-02	2.4000E-03
13	*****	*****	5.0000E-05	4.0000E-04	2.6500E-03	1.2100E-02	3.7250E-02	7.1650E-02	7.1150E-02	1.6500E-02
14	*****	*****	*****	1.5000E-04	1.0000E-03	5.3000E-03	1.9400E-02	4.8250E-02	7.3650E-02	5.2650E-02
15	*****	*****	*****	5.0000E-05	4.0000E-04	2.1500E-03	9.3000E-03	2.8050E-02	5.7000E-02	6.8600E-02
16	*****	*****	*****	*****	1.5000E-04	8.5000E-04	4.2000E-03	1.4800E-02	3.7050E-02	6.1700E-02
17	*****	*****	*****	*****	5.0000E-05	3.0000E-04	1.8500E-03	7.3000E-03	2.1400E-02	4.5050E-02
18	*****	*****	*****	*****	*****	1.5000E-04	7.5000E-04	3.4000E-03	1.1450E-02	2.8700E-02
19	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

VV	10	11	12	13	14	15	16	17	18	19
V										
0	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
2	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
3	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
4	3.5000E-04	*****	*****	*****	*****	*****	*****	*****	*****	*****
5	1.0700E-01	6.5000E-04	*****	*****	*****	*****	*****	*****	*****	*****
6	1.1070E-01	1.7650E-02	1.2500E-03	*****	*****	*****	*****	*****	*****	*****
7	2.7275E-01	1.4315E-01	2.7000E-02	2.1500E-03	1.0000E-04	*****	*****	*****	*****	*****
8	3.2050E-02	2.6055E-01	1.7620E-01	3.9100E-02	3.5500E-03	1.5000E-04	*****	*****	*****	*****
9	1.2420E-01	6.4500E-03	2.3455E-01	2.0660E-01	5.3650E-02	5.5000E-03	2.5000E-04	*****	*****	*****
10	2.5000E-04	1.2965E-01	5.5000E-04	1.9850E-01	2.3255E-01	7.1100E-02	8.2500E-03	3.5000E-04	*****	*****
11	6.7800E-02	9.7500E-03	1.1835E-01	6.0750E-02	1.5685E-01	2.5195E-01	9.0900E-02	1.1800E-02	6.0000E-04	*****
12	7.2050E-02	3.9750E-02	2.9900E-02	9.5150E-02	3.1700E-02	1.1455E-01	2.6465E-01	1.1280E-01	1.6350E-02	*****
13	1.4250E-02	7.6850E-02	1.6550E-02	5.2750E-02	6.6600E-02	5.7550E-02	7.5450E-02	2.6925E-01	1.3565E-01	*****
14	3.5000E-03	3.1250E-02	6.9850E-02	3.2000E-03	7.1750E-02	3.8850E-02	8.2450E-02	4.3400E-02	2.6565E-01	*****
15	3.2750E-02	7.5000E-04	4.7100E-02	5.4350E-02	9.5000E-04	8.2500E-02	1.7000E-02	1.0195E-01	2.0200E-02	*****
16	5.7600E-02	1.5750E-02	6.7000E-03	5.7350E-02	3.5650E-02	8.4000E-03	8.3300E-02	4.2000E-03	1.1325E-01	*****
17	6.1450E-02	4.2900E-02	4.6000E-03	1.8200E-02	5.5700E-02	1.8150E-02	2.1950E-02	7.5050E-02	1.1000E-03	*****
18	5.0650E-02	5.6000E-02	2.7050E-02	7.5000E-04	3.1450E-02	5.4150E-02	5.9500E-03	3.7150E-02	6.0200E-02	*****
19	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

DIATOMIC TRANSITION C2SWAN INDEX NO. SPECIFYING SUBROUTINE USED IN CALC. 1 NUMBER SPECIFYING DATA LOCATION ON TAPE 3

SPECTROGRAPHIC CONSTANTS FROM BALLIK AND RAMSAY ASTROPHYS J. 137,1963
EXCEPT FOR SPIN COUPLING CONSTANTS WHICH WERE TAKEN FROM HERZBERG.
RKR FRANCK-CONDON FACTORS FROM SPINDLER JQSRT VOL. 5, P 195 (1965).
THIS TRANSITION COMPUTED IN SUBROUTINE ZERO.

LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT
C.	0.0	10	6.0019

SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY CEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
UPPER STATE -16.90	1	0.0000000E-38	0.0000000E-38	0.2950000E 05	0.1266000E-07
LOWER STATE -16.40	1	0.0000000E-38	0.0000000E-38	0.4890000E 05	0.1311900E-07

ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEZE	WEYE	WEZE	BE	ALPHA E
UPPER STATE 6	2.0022500E 04	1.7882200E 03	1.6440000E 01	-5.0670000E-01	0.0000000E-39	1.7527000E 00	1.6080000E-02
LOWER STATE 6	7.1624000E 02	1.6413500E 03	1.1670000E 01	0.0000000E-39	0.0000000E-39	1.6324600E 00	1.6610000E-02
1	5.5034600E 04	1.6715000E 03	4.0020000E 01	2.4000000E-01	0.0000000E-39	1.7930000E 00	4.2100000E-02
1	4.3240230E 04	1.8295700E 03	1.3970000E 01	0.0000000E-39	0.0000000E-39	1.8334000E 00	2.0400000E-02
6	4.0766650E 04	1.1065600E 03	3.5260000E 01	2.8000000E 00	0.0000000E-39	1.1922000E 00	2.4200000E-02
2	3.4261900E 04	1.8091000E 03	1.5810000E 01	-4.0200000E 00	0.0000000E-39	1.7834000E 00	1.8000000E-02
3	1.3312100E 04	1.9616000E 03	1.3850000E 01	0.0000000E-39	0.0000000E-39	1.8700000E 00	0.0000000E-39
2	8.3910000E 03	1.6083500E 03	1.2078000E 01	-1.0000000E-02	0.0000000E-39	1.6163400E 00	1.6880000E-02
3	6.4342700E 03	1.4704500E 03	1.1190000E 01	2.0000000E-02	0.0000000E-39	1.4985200E 00	1.6340000E-02
1	0.0000000E-39	1.8547100E 03	1.3340000E 01	-1.7200000E-01	0.0000000E-39	1.8198400E 00	1.7650000E-02

FRANCK-CONDON FACTOR

VV	C	1	2	3	4	5	6	7	8	9
V										
0	7.2130E-01	2.2060E-C1	4.7600E-C2	8.8000E-03	1.5000E-03	2.0000E-04	*****	*****	*****	*****
1	2.5060E-01	3.3710E-C1	2.8030E-C1	5.9900E-02	2.5400E-02	5.4000E-03	1.0000E-03	2.0000E-04	*****	*****
2	2.7200E-02	3.7420E-C1	1.3810E-C1	2.6210E-01	1.3770E-C1	4.5300E-02	1.1900E-02	2.7000E-03	6.0000E-04	1.0000E-04
3	8.0000E-C4	6.5900E-02	4.2550E-C1	4.7700E-02	2.1120E-01	1.5720E-01	6.4700E-02	2.0200E-02	5.2000E-03	1.2000E-03
4	*****	2.2000E-03	1.0550E-C1	4.4460E-01	1.4300E-02	1.5760E-01	1.5920E-01	7.8200E-02	2.7900E-02	8.1000E-03
5	*****	*****	2.8000E-C3	1.3410E-01	4.5850E-01	4.6000E-03	1.1370E-01	1.5250E-01	8.3700E-02	3.4000E-02
6	*****	*****	2.0000E-C4	1.9000E-03	1.4920E-01	4.8310E-01	4.2000E-C3	8.0400E-02	1.4060E-01	8.5800E-02
7	*****	*****	8.0000E-04	1.0000E-04	1.4130E-01	5.1920E-01	1.0300E-02	5.6800E-02	1.3220E-01	3.6700E-02
8	*****	*****	*****	2.1000E-03	1.7000E-03	1.1030E-01	5.6020E-01	3.0600E-02	3.6700E-02	7.9600E-02
9	*****	*****	*****	*****	3.2000E-03	1.2100E-02	5.8500E-02	5.8190E-C1	7.9600E-02	*****
10	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
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VV	10	11	12	13	14	15	16	17	18	19
V										
C	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
1	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
2	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
3	2.0000E-C4	*****	*****	*****	*****	*****	*****	*****	*****	*****
4	2.0000E-C3	4.0000E-04	1.0000E-C4	*****	*****	*****	*****	*****	*****	*****
5	1.8000E-02	2.9000E-C3	6.0000E-C4	1.0000E-04	*****	*****	*****	*****	*****	*****
6	3.7500E-C2	1.2600E-C2	3.5000E-C3	8.0000E-04	*****	*****	*****	*****	*****	*****
7	8.1600E-02	3.8900E-C2	1.3500E-C2	3.9000E-03	*****	*****	*****	*****	*****	*****
8	1.2940E-01	7.2700E-C2	3.7900E-C2	1.3200E-02	*****	*****	*****	*****	*****	*****
9	1.8400E-C2	1.3400E-C1	5.9500E-C2	3.5500E-C2	*****	*****	*****	*****	*****	*****
10	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
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DIATOMIC TRANSITION
OH3060

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
3

NUMBER
SPECIFYING
DATA LOCATION
ON TAPE
4

SPECTROGRAPHIC CONSTANTS FROM HERZBERG.
MORSE FRANCK-CONDON FACTORS ASTROPHYS J. P 55 (1955)
THIS TRANSITION COMPUTED IN SUBROUTINE S2 P12.

	LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR MONONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT				
	0.	0.0	2	0.9484				
	SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM		
UPPER STATE	0.00	C	0.0000000E-38	0.0000000E-38	0.0000000E-38	C.1C12100E-07		
LOWER STATE	139.99	1	0.0000000E-38	0.0000000E-38	0.3510000E 05	C.9706000E-08		
	ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEZE	WEYE	WEZE	BE	ALPHA E
UPPER STATE	2	3.268250CE 04	3.180560CE 03	9.4930000E 01	-6.47C0000E-01	0.0000000E-39	1.735500CE 01	8.07C0000E-01
LOWER STATE	4	0.0000000E-39	3.7352100E 03	8.2810000E 01	0.0000000E-39	0.0000000E-39	1.8871000E 01	7.14C0000E-01

FRANCK-CONDON FACTOR

VV	0	1	2	3	4	5	6	7	8	9
V										
0	5.0700E-01	8.9000E-02	3.0000E-03	*****	*****	*****	*****	*****	*****	*****
1	8.6000E-02	7.1600E-01	1.8600E-01	1.2000E-02	*****	*****	*****	*****	*****	*****
2	6.0000E-03	1.6500E-01	5.1400E-01	2.8000E-01	3.2000E-02	*****	*****	*****	*****	*****
3	*****	2.3000E-02	2.3700E-01	3.2100E-01	3.2900E-01	*****	*****	*****	*****	*****
4	*****	3.0000E-03	5.4000E-02	2.5300E-01	*****	*****	*****	*****	*****	*****
5	*****	*****	7.0000E-03	*****	*****	*****	*****	*****	*****	*****
6	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
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VV	10	11	12	13	14	15	16	17	18	19
V										
0	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
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18	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
19	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

DIATOMIC
TRANSITION
CO 4+

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
2

NUMBER
SPECIFYING
DATA LOCATION
ON TAPE
5

SPECTROGRAPHIC CONSTANTS FROM HERZBERG.
MORSE FRANK-CONDON FACTORS BY NICHOLLS
THIS TRANSITION COMPUTED IN SUBROUTINE ONE

REF JQSRT 2 (1962)

LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT
0.	0.0	11	6.8584

UPPER STATE	SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
UPPER STATE	0.00	1	0.0000000E-38	0.0000000E-38	0.0000000E-38	0.1235100E-07
LOWER STATE	0.00	0	0.0000000E-38	0.0000000E-38	0.8960000E 05	0.1128190E-07

UPPER STATE	LOWER STATE	ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEZE	WEYE	WEZE	BE	ALPHA E
2	1	2	6.5074800E 04	1.5156100E 03	1.7250500E 01	0.0000000E-39	0.0000000E-39	1.6116000E 00	2.2290000E-02
1	2	1	0.0000000E-39	2.1702100E 03	1.3461000E 01	3.0800000E-02	0.0000000E-39	1.9313900E 00	1.7485000E-02
3	1	2	5.9805000E 04	2.1120000E 03	1.5800000E 02	0.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39
1	3	1	9.3157800E 04	0.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	1.9563000E 00	0.0000000E-39
1	1	1	5.2928000E 04	2.1340000E 03	0.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39
1	1	1	9.1926000E 04	2.1330000E 03	0.0000000E-39	0.0000000E-39	0.0000000E-39	1.9422000E 00	0.0000000E-39
1	1	1	8.6948000E 04	2.0820700E 03	0.0000000E-39	0.0000000E-39	0.0000000E-39	1.9610000E 00	2.7000000E-02
3	1	1	8.3804000E 04	2.1980000E 03	0.0000000E-39	0.0000000E-39	0.0000000E-39	2.0750000E 00	3.3000000E-02
6	1	1	6.2259400E 04	1.1377900E 03	7.6240000E 00	-1.1250000E-01	0.0000000E-39	1.2615000E 00	1.7000000E-02
3	1	1	5.5901000E 04	1.2180000E 03	9.5000000E 00	0.0000000E-39	0.0000000E-39	1.3310000E 00	1.6000000E-02
6	1	1	4.8687500E 04	1.7392500E 03	1.4470000E 01	0.0000000E-39	0.0000000E-39	1.6810000E 00	1.9300000E-02

FRANK-CONDON FACTOR

VV	C	1	2	3	4	5	6	7	8	9
0	1.1219E-01	2.6087E-01	2.8477E-01	1.9629E-01	9.6040E-02	3.5535E-02	1.0340E-02	2.4282E-03	4.6859E-04	7.5264E-05
1	2.1614E-01	1.5487E-01	3.0508E-03	7.6435E-02	1.9313E-01	1.8569E-01	1.0829E-01	4.4465E-02	1.3804E-02	3.3745E-03
2	2.2597E-01	1.2179E-02	9.0126E-02	1.1607E-01	5.0832E-03	5.7179E-02	1.6502E-01	1.6681E-01	9.9629E-02	4.1314E-02
3	1.8128E-01	2.0493E-02	1.1704E-01	6.4536E-04	8.9569E-02	8.4157E-02	4.7128E-04	6.7660E-02	1.5884E-01	1.4862E-01
4	1.1879E-01	6.7285E-02	3.4433E-02	5.7630E-02	6.6561E-02	6.1711E-03	9.8034E-02	5.1406E-02	2.7202E-03	8.9110E-02
5	6.8846E-02	1.2304E-01	3.2357E-04	9.1254E-02	1.3841E-05	8.2359E-02	2.2684E-02	3.1553E-02	9.4377E-02	2.1092E-02
6	3.6675E-02	1.1603E-01	3.2109E-02	4.2201E-02	4.2898E-02	4.2265E-02	2.1776E-02	7.2885E-02	5.9304E-04	6.3519E-02
7	1.8429E-02	8.8057E-02	7.3469E-02	2.2336E-03	7.3886E-02	4.2668E-05	6.9877E-02	2.9021E-03	5.8181E-02	3.7499E-02
8	8.8974E-03	5.8371E-02	9.0572E-02	5.8554E-03	4.4622E-02	3.2779E-02	2.5742E-02	3.0612E-02	4.2672E-02	9.8388E-03
9	4.1842E-03	3.5370E-02	8.4527E-02	4.0627E-02	7.5687E-03	6.0808E-02	3.8286E-05	5.8344E-02	1.6689E-05	5.8879E-02
10	1.9367E-03	2.0162E-02	6.6327E-02	6.4755E-02	1.4618E-03	4.5052E-02	2.4181E-02	2.3731E-02	3.2522E-02	2.3741E-02
11	8.8941E-04	1.1024E-02	4.6641E-02	7.1751E-02	1.9480E-02	1.4504E-02	4.9695E-02	1.1030E-05	4.9442E-02	1.0943E-03
12	4.0787E-04	5.8643E-03	3.0446E-02	6.5086E-02	4.1768E-02	1.7143E-04	4.4180E-02	1.6298E-02	2.1594E-02	3.0204E-02
13	1.8773E-04	3.0666E-03	1.8881E-02	5.2041E-02	5.5313E-02	6.7201E-03	2.0995E-02	3.9190E-02	4.2287E-04	4.2877E-02
14	8.7084E-05	1.5891E-03	1.1304E-02	3.8223E-02	5.7629E-02	2.3102E-02	3.3642E-03	4.1680E-02	9.2001E-03	2.1882E-02
15	4.0846E-05	8.2117E-04	6.6118E-03	2.6471E-02	5.1936E-02	3.7973E-02	7.3801E-04	2.6615E-02	2.8617E-02	1.9365E-03
16	1.9425E-05	4.2525E-04	3.8121E-03	1.7597E-02	4.2528E-02	4.5527E-02	9.4788E-03	9.4220E-03	3.6896E-02	3.5232E-03
17	9.3667E-06	2.2157E-04	2.1816E-03	1.1373E-02	3.2596E-02	4.6731E-02	2.1795E-02	6.1450E-04	3.0143E-02	1.8049E-02
18	4.6172E-06	1.1653E-04	1.2459E-03	7.2159E-03	2.3851E-02	4.2574E-02	3.1818E-02	1.6937E-03	1.6581E-02	2.9379E-02
19	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

VV	10	11	12	13	14	15	16	17	18	19
0	1.0151E-05	1.1568E-06	1.1181E-07	5.1869E-09	6.4215E-10	3.7782E-11	1.8874E-12	9.6394E-14	1.9682E-15	1.7458E-16
1	6.6637E-04	1.0812E-04	1.4579E-05	1.6462E-06	1.5635E-07	1.2525E-08	8.4721E-10	4.8179E-11	2.2816E-12	8.8683E-14
2	1.2831E-02	3.1152E-03	6.0724E-04	5.6710E-05	1.2731E-05	1.3957E-06	1.2800E-07	9.8388E-09	6.3250E-10	3.4137E-11
3	8.4545E-02	3.3725E-02	1.0112E-02	2.3717E-03	4.4621E-04	6.8445E-05	8.6524E-06	9.0748E-07	7.9258E-08	5.7731E-09
4	1.5679E-01	1.2914E-01	6.7610E-02	2.5283E-02	7.1696E-03	1.5570E-03	2.8572E-04	4.1658E-05	4.9963E-06	4.9572E-07
5	1.8021E-02	1.1259E-01	1.5095E-01	1.0784E-01	5.1173E-02	1.7696E-02	4.6884E-03	9.8077E-04	1.6515E-04	2.2666E-05
6	7.2827E-02	2.4331E-03	4.5471E-02	1.3211E-01	1.3855E-01	8.5849E-02	3.6707E-02	1.1654E-02	2.8628E-03	5.5819E-04
7	1.0104E-02	8.2806E-02	4.0479E-02	2.7402E-03	7.8643E-02	1.4142E-01	1.2017E-01	6.4922E-02	2.4980E-02	7.2532E-03
8	6.8218E-02	6.0762E-03	4.0752E-02	7.7972E-02	1.1842E-02	2.2424E-02	1.0892E-01	1.3911E-01	9.8285E-02	4.6607E-02
9	5.5671E-03	4.3499E-02	4.4543E-02	2.4546E-03	6.9276E-02	5.2619E-02	1.8350E-05	5.4755E-02	1.2915E-01	1.2656E-01
10	2.4797E-02	4.1657E-02	4.7082E-03	6.2178E-02	1.2255E-02	2.6202E-02	7.6757E-02	2.1822E-02	1.0029E-02	8.9341E-02
11	4.9911E-02	5.7511E-06	5.1872E-02	8.4925E-03	3.3523E-02	4.8135E-02	1.3307E-04	5.7040E-02	6.0064E-02	2.2404E-02
12	1.4378E-02	3.1435E-02	2.0623E-02	2.0729E-02	4.0579E-02	1.7866E-03	5.6287E-02	1.8132E-02	1.6162E-02	7.2885E-02
13	1.7179E-03	4.1004E-02	2.1272E-03	4.4591E-02	6.1243E-06	4.6549E-02	1.1148E-02	2.5596E-02	5.0261E-02	4.4292E-04
14	2.5544E-02	1.0672E-02	3.1550E-02	1.0101E-02	2.9406E-02	1.9578E-02	1.6848E-02	4.0513E-02	4.4129E-04	5.0304E-02
15	3.7613E-02	1.2081E-03	3.4831E-02	4.0014E-03	3.5446E-02	2.3548E-03	4.1117E-02	1.5983E-04	4.1675E-02	1.4535E-02
16	2.3565E-02	1.5485E-02	1.0152E-02	2.8332E-02	6.0848E-03	3.0450E-02	8.6642E-03	2.6350E-02	2.0329E-02	1.2562E-02
17	5.1274E-03	3.2376E-02	2.6512E-04	3.1077E-02	3.7993E-03	2.9198E-02	4.8212E-03	3.2361E-02	1.7042E-02	3.8687E-02
18	3.2516E-04	2.5475E-02	1.2637E-02	1.1864E-02	2.3360E-02	5.3800E-03	2.7723E-02	4.6775E-03	2.7916E-02	9.2564E-03
19	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

DIATOMIC
TRANSITION
N2+ 1-

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
1

NUMBER
SPECIFYING
DATA LOCATION
ON TAPE
6

SPECTROGRAPHIC CONSTANTS FROM HERZBERG.
MORSE FRANCK-CONDON FACTORS
NBS VCL 65A 1961 P451
THIS TRANSITION COMPUTED IN SUBROUTINE ZERO

LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT
1.	1.0	3	7.0036

SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY CEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
UPPER STATE C.00	C	0.0000000E-38	0.0000000E-38	0.0000000E-38	0.1075000E-07
LOWER STATE 0.00	C	0.0000000E-38	0.0000000E-38	0.7039000E 05	0.1116200E-07

ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEXE	WEYE	WEZE	BE	ALPHA E
UPPER STATE 2	2.5461500E 04	2.4198400E 03	2.3190000E 01	-5.3750000E-01	0.0000000E-39	2.0830000E 00	1.9500000E-02
LOWER STATE 2	0.0000000E-39	2.2071900E 03	1.6136000E 01	-4.0000000E-02	0.0000000E-39	1.9322000E 00	2.0200000E-02
2	6.4622000E 04	2.0500000E 03	0.0000000E-39	0.0000000E-39	0.0000000E-39	1.6500000E 00	5.0000000E-02

FRANCK-CONDON FACTOR

VV	C	1	2	3	4	5	6	7	8	9
0	6.5094E-01	2.5883E-01	7.0162E-02	1.5957E-02	3.2972E-03	6.3420E-04	1.1549E-04	1.9998E-05	3.2805E-06	5.0335E-07
1	3.0144E-01	2.2260E-01	2.8598E-01	1.3242E-01	4.2726E-02	1.1403E-02	2.6998E-03	5.8613E-04	1.1849E-04	2.2393E-05
2	4.5371E-02	4.0559E-01	5.0646E-02	2.2501E-01	1.6535E-01	7.1133E-02	2.2623E-02	6.6908E-03	1.6951E-03	3.9336E-04
3	2.2475E-03	1.0562E-01	4.1372E-01	2.1005E-03	1.5566E-01	1.7060E-01	9.4514E-02	3.8008E-02	1.2612E-02	3.6675E-03
4	1.4521E-05	6.9353E-03	1.6604E-01	3.7922E-01	6.7256E-03	5.2901E-02	1.5692E-01	1.0964E-01	5.2363E-02	2.0033E-02
5	4.6340E-07	3.9858E-05	1.3395E-02	2.2051E-01	3.3100E-01	2.9248E-02	4.8153E-02	1.3327E-01	1.1606E-01	6.4883E-02
6	9.4619E-09	3.0877E-06	5.7286E-05	2.0691E-02	2.6731E-01	2.8304E-01	5.3307E-02	2.0444E-02	1.0647E-01	1.1499E-01
7	6.4377E-10	3.4169E-08	1.1319E-05	4.9298E-05	2.7894E-02	3.0677E-01	2.4145E-01	7.2364E-02	5.6387E-03	8.0835E-02
8	4.1958E-13	5.7552E-09	4.9506E-06	3.0055E-05	1.8070E-05	3.4188E-02	3.4009E-01	2.0830E-01	8.4684E-02	4.7434E-04
9	1.2746E-12	3.8766E-12	2.6591E-08	1.7424E-08	6.4203E-05	1.0666E-06	3.8904E-02	3.6856E-01	1.8373E-01	9.0654E-02
10	3.5487E-14	1.0275E-11	1.7096E-10	8.3563E-08	3.2950E-08	1.1610E-04	8.0941E-05	4.1527E-02	3.9326E-01	1.6717E-01
11	2.8767E-16	6.9997E-13	3.8767E-11	1.6762E-09	1.5686E-07	6.7150E-07	1.8230E-04	3.8725E-04	4.1704E-02	4.1493E-01
12	5.2594E-16	2.4906E-15	5.5598E-12	7.8486E-11	9.1842E-09	3.5533E-07	3.5224E-06	2.5089E-04	1.0871E-03	3.9276E-02
13	7.4212E-20	9.9105E-16	1.0051E-13	2.7547E-11	5.7016E-11	3.5189E-08	4.9932E-07	1.1720E-05	3.0102E-04	2.3614E-03
14	1.7188E-16	8.9552E-17	1.3821E-15	9.9713E-13	9.4783E-11	1.3391E-11	1.0410E-07	4.7645E-07	3.0048E-05	3.0712E-04
15	1.8407E-16	4.0381E-17	2.6642E-15	3.0960E-15	7.6533E-12	2.2485E-10	1.1384E-09	2.4797E-07	2.0416E-07	6.3998E-05
16	1.8155E-17	5.4575E-18	2.8290E-15	6.5616E-15	2.0529E-14	3.6688E-11	3.6122E-10	8.9261E-09	4.8200E-07	1.5601E-08
17	9.5257E-17	1.3459E-16	1.3306E-15	1.5689E-15	5.3219E-14	1.1348E-12	1.2484E-10	2.8360E-10	3.8957E-08	7.5533E-07
18	3.2282E-16	6.4620E-16	2.7374E-17	3.0826E-15	7.6808E-15	4.8177E-14	8.8436E-12	3.2815E-10	2.0518E-15	1.2246E-07
19	3.0466E-16	6.7846E-16	1.1417E-16	2.9053E-15	3.1337E-17	7.9994E-14	3.1504E-14	4.3885E-11	6.1538E-10	1.8664E-09

VV	10	11	12	13	14	15	16	17	18	19
0	7.0274E-08	8.4194E-09	7.4706E-10	2.7246E-11	1.5572E-12	5.7438E-12	4.0732E-12	1.9329E-12	7.4934E-13	2.4709E-13
1	3.9213E-06	6.2862E-07	8.7554E-08	9.5331E-09	5.6580E-10	2.7584E-13	4.1016E-11	3.8757E-11	2.1156E-11	9.2253E-12
2	8.4449E-05	1.6754E-05	3.0305E-06	4.8313E-07	6.2656E-08	5.2243E-09	5.9097E-11	1.2927E-10	1.8980E-10	1.2444E-10
3	9.6386E-04	2.3237E-04	5.1559E-05	1.0440E-05	1.8810E-06	2.8382E-07	3.0499E-08	1.1388E-09	1.9308E-10	5.9679E-10
4	6.5985E-03	1.9422E-03	5.2074E-04	1.2807E-04	2.8771E-05	5.7951E-06	9.9985E-07	1.3165E-07	8.8002E-09	5.3633E-11
5	2.8257E-02	1.0429E-02	3.4058E-03	1.0071E-03	2.7242E-04	6.7369E-05	1.5032E-05	2.9233E-06	4.5566E-07	4.4113E-08
6	7.4424E-02	3.6515E-02	1.4962E-02	5.3781E-03	1.7413E-03	5.1455E-04	1.3912E-04	3.4114E-05	7.3925E-06	1.3305E-06
7	1.0837E-01	8.0508E-02	4.4113E-02	1.9912E-02	7.8225E-03	2.7556E-03	8.8413E-04	2.5973E-04	6.5513E-05	1.6626E-05
8	5.6649E-02	5.8214E-02	8.3188E-02	5.0528E-02	2.4953E-02	1.0647E-02	4.0574E-03	1.4059E-03	4.4632E-04	1.2957E-04
9	5.5515E-04	4.0751E-02	8.6284E-02	8.2879E-02	5.5439E-02	2.5771E-02	5.8721E-02	1.2721E-02	5.6271E-03	2.0953E-03
10	9.1407E-02	3.6040E-03	2.7101E-02	7.3930E-02	8.0178E-02	5.7471E-02	3.4099E-02	1.6889E-02	7.4191E-03	2.9555E-03
11	1.5792E-01	8.8180E-02	7.8956E-03	1.7195E-02	6.2084E-02	7.5740E-02	6.0410E-02	3.7741E-02	1.5954E-02	9.3675E-03
12	4.3379E-01	1.5540E-01	8.2045E-02	1.2382E-02	1.0343E-02	5.1312E-02	7.0185E-02	6.0656E-02	4.0577E-02	2.2892E-02
13	3.4320E-02	4.4957E-01	1.5933E-01	7.3838E-02	1.6506E-02	5.8379E-03	4.1892E-02	6.4044E-02	5.5684E-02	4.2558E-02
14	4.3643E-03	2.7223E-02	4.6145E-01	1.6967E-01	6.4180E-02	2.0049E-02	3.0433E-03	3.3901E-02	5.7743E-02	5.7746E-02
15	2.4992E-04	7.1648E-03	1.8762E-02	4.6808E-01	1.8661E-01	5.3547E-02	2.3101E-02	1.4302E-03	2.7284E-02	5.1592E-02
16	1.1714E-04	1.3548E-04	1.0676E-02	1.0178E-02	4.6761E-01	2.1044E-01	4.2359E-02	2.5526E-02	5.8439E-04	2.1907E-02
17	1.3451E-06	1.6672E-04	2.0326E-05	1.4566E-02	3.2073E-03	4.5788E-01	2.4131E-01	3.1069E-02	2.7824E-02	1.9790E-04
18	9.0082E-07	7.5652E-06	2.5870E-04	3.5495E-05	1.8313E-02	1.9948E-05	4.3662E-01	2.7903E-01	2.0265E-02	3.0199E-07
19	3.0166E-07	6.8357E-07	2.4387E-05	3.0557E-04	3.9546E-04	2.1029E-02	3.0089E-03	4.0194E-01	3.2267E-01	1.0750E-02

DIATOMIC
TRANSITION
N2 1+

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
2

NUMBER
SPECIFYING
DATA LOCATION
ON TAPE
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SPECTROGRAPHIC CONSTANTS FROM HERZBERG
MORSE FRANK CONDON FACTORS
NBS VOL 65 A NC 5 1961 PAGE 451
THIS TRANSITION COMPUTED IN SUBROUTINE CNE

LINE ALTERNATION FACTOR		NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES		NUMBER OF ELECTRONIC LEVELS		REDUCED ATOMIC WEIGHT	
1.		1.0		10		7.0038	
SPIN COUPLING CONSTANT		QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS		ROTATIONAL CONSTANT DE, 1/CM		DISSOCIATION ENERGY DEZERO, 1/CM	
UPPER STATE		1		0.0000000E-38		C.0000000E-38	
LOWER STATE		0		0.0000000E-38		0.0000000E-38	
ELECTRONIC DEGENERACY		ELECTRONIC TERM ENERGY		ROTATIONAL CONSTANT ETA, 1/CM		INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM	
UPPER STATE		WE		WEYE		BE	
LOWER STATE		WE		WEZE		ALPHA E	
6	5.562630CE 04	1.7341100E 03	1.4470000E 01	C.0000000E-39	C.0000000E-39	1.6380000E 00	1.8400000E-02
3	5.0206000E 04	1.4603700E 03	1.3891000E 01	-2.5000000E-02	0.0000000E-39	1.4400000E 00	1.3000000E-02
1	5.9327000E 04	6.7000000E 02	C.0000000E-39	C.0000000E-39	C.0000000E-39	1.4600000E 00	0.0000000E-39
3	5.7584000E 04	C.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39
3	5.5770000E 04	2.1845000E 03	C.0000000E-39	C.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39
6	8.914730CE 04	2.0351000E 03	1.7080000E 01	-2.1500000E 00	0.0000000E-39	1.8259000E 00	1.9700000E-02
2	6.9290000E 04	1.6520100E 03	1.2791000E 01	-3.4590000E-01	0.0000000E-39	1.6370000E 00	2.2400000E-02
2	6.3943000E 04	1.5601000E 03	1.1900000E 01	0.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39
1	6.0000000E 04	1.5270000E 03	1.1500000E 01	0.0000000E-39	0.0000000E-39	1.4800000E 00	1.5000000E-02
1	C.0000000E-39	2.3596100E 03	1.4456000E 01	7.5100000E-03	-5.0900000E-04	2.0100000E 00	1.8700000E-02

FRANK-CONDON FACTOR

VV	C	1	2	3	4	5	6	7	8	9
V										
0	3.3816E-01	3.2480E-01	1.8996E-01	8.8567E-02	3.6486E-02	1.3990E-02	5.1465E-03	1.8513E-03	6.5953E-04	2.3477E-04
1	4.0645E-01	2.3100E-01	1.0321E-01	1.7820E-01	1.4502E-01	8.6473E-02	4.3670E-02	1.9997E-02	8.6259E-03	3.5891E-03
2	1.5746E-01	2.1203E-01	1.1320E-01	1.2048E-03	7.7240E-02	1.2750E-01	1.1271E-01	7.4955E-02	4.2471E-02	2.1815E-02
3	5.0143E-02	2.9871E-01	3.8683E-02	1.6230E-01	3.2267E-02	9.0504E-03	6.9100E-02	1.0094E-01	9.0789E-02	6.4061E-02
4	1.1505E-03	1.3180E-01	2.7381E-01	1.8081E-01	1.1388E-01	8.8227E-02	5.2273E-03	1.7977E-02	6.3607E-02	2.4543E-02
5	5.8713E-04	2.7286E-02	2.1065E-01	2.6054E-01	8.3053E-02	1.6404E-01	3.1711E-03	8.0781E-02	6.9671E-02	1.2893E-02
6	2.6156E-05	2.9248E-03	6.1481E-02	1.8566E-02	2.7061E-01	1.6163E-02	1.2905E-01	6.7482E-03	3.9461E-02	7.7327E-02
7	5.6982E-07	1.6132E-04	8.4620E-03	1.0650E-01	2.7061E-01	1.6163E-02	1.2905E-01	6.7482E-03	3.9461E-02	7.7327E-02
8	4.7221E-09	4.1737E-06	5.6752E-04	1.8566E-02	1.5609E-01	2.4380E-01	2.7659E-05	1.1586E-01	3.6330E-02	8.3601E-03
9	6.5075E-12	3.9626E-08	1.7188E-05	1.4947E-03	3.4197E-02	2.0292E-01	1.6185E-01	1.6939E-02	7.8622E-02	6.7727E-02
10	2.7802E-15	6.0552E-11	1.8482E-07	5.2408E-05	3.2741E-03	5.5689E-02	2.4021E-01	1.2991E-01	5.2188E-02	3.7645E-02
11	8.1140E-16	3.3224E-14	3.0349E-10	6.3216E-07	1.3176E-04	6.2985E-03	8.2650E-02	2.6301E-01	7.2055E-02	8.7792E-02
12	2.5148E-16	5.0349E-16	2.1376E-13	1.0121E-09	1.7690E-06	2.8895E-04	1.0992E-02	1.1398E-01	2.6878E-01	2.8566E-02
13	5.5625E-17	1.6620E-16	4.3337E-16	1.0512E-12	3.2357E-09	4.2896E-06	5.7172E-04	1.7773E-02	2.6878E-01	2.8566E-02
14	3.4245E-16	4.4756E-17	4.5421E-16	5.7232E-16	4.0476E-12	8.1628E-09	9.3348E-06	1.0436E-03	2.7016E-02	1.8258E-01
15	1.7005E-16	2.5344E-16	2.7160E-17	4.1387E-16	2.8052E-15	1.2846E-11	1.8385E-08	1.8657E-05	1.7849E-01	3.9015E-02
16	5.1720E-18	7.4160E-17	2.2234E-16	4.9038E-17	6.3948E-17	4.5515E-14	3.4427E-11	3.7813E-08	3.4803E-05	2.8927E-03
17	2.0782E-16	1.5676E-17	2.1122E-16	5.4009E-16	2.1696E-15	2.4366E-15	2.1664E-13	8.5321E-11	7.2030E-08	6.1314E-05
18	1.8889E-16	1.2423E-16	2.4354E-17	9.1758E-17	1.2590E-16	3.5570E-16	3.0869E-17	4.8996E-13	1.9965E-10	1.2872E-07
19	1.0678E-17	1.1379E-16	1.9019E-17	2.6078E-16	9.9179E-16	3.8594E-15	4.2273E-15	8.3215E-15	1.2193E-12	4.2255E-10

VV	10	11	12	13	14	15	16	17	18	19
V										
0	8.4031E-05	3.0383E-05	1.1135E-05	4.1473E-06	1.5729E-06	6.0831E-07	2.4019E-07	*****	*****	*****
1	1.4631E-03	5.9070E-04	2.3802E-04	9.6271E-05	3.9251E-05	1.6185E-05	6.7658E-06	*****	*****	*****
2	1.0529E-02	4.8845E-03	2.2119E-03	5.8835E-04	4.3920E-04	1.9525E-04	8.7217E-05	*****	*****	*****
3	3.5171E-02	2.1871E-02	1.1508E-02	5.8243E-03	2.8759E-03	1.3995E-03	6.7625E-04	*****	*****	*****
4	7.5106E-02	5.5103E-02	3.5667E-02	2.1275E-02	1.2016E-02	6.5421E-03	2.4791E-03	*****	*****	*****
5	5.8198E-02	7.0564E-02	6.3384E-02	4.7549E-02	3.2525E-02	2.0514E-02	1.2313E-02	*****	*****	*****
6	2.4600E-03	2.8059E-02	5.2611E-02	6.0354E-02	5.4340E-02	4.2250E-02	2.9867E-02	*****	*****	*****
7	3.8328E-02	2.7384E-03	6.4003E-03	2.9121E-02	4.7031E-02	5.2119E-02	4.7183E-02	*****	*****	*****
8	6.0700E-02	5.7211E-02	1.8520E-02	8.6772E-05	9.5049E-03	2.8339E-02	4.1643E-02	*****	*****	*****
9	3.1940E-04	3.3048E-02	5.6448E-02	3.7269E-02	7.9625E-03	3.6806E-04	1.1202E-02	*****	*****	*****
10	8.3700E-02	1.3068E-02	9.5758E-03	4.6033E-02	4.8138E-02	2.2815E-02	3.0276E-03	*****	*****	*****
11	9.0118E-03	7.8966E-02	3.5274E-02	6.6872E-05	2.5442E-02	4.6325E-02	3.5766E-02	*****	*****	*****
12	1.1086E-01	2.6171E-05	5.8457E-02	5.4227E-02	5.7104E-03	7.8299E-03	3.3974E-02	*****	*****	*****
13	4.6872E-03	1.1561E-01	9.3424E-03	3.2354E-02	6.1513E-02	2.0820E-02	1.3633E-04	*****	*****	*****
14	2.3145E-01	7.7329E-04	1.0292E-01	2.9820E-02	1.0861E-02	5.5268E-02	3.6818E-02	*****	*****	*****
15	2.1544E-01	1.9452E-01	1.3301E-02	7.8250E-02	5.2260E-02	5.5460E-04	3.9360E-02	*****	*****	*****
16	5.3547E-02	2.4432E-01	1.5158E-01	3.6327E-02	4.9346E-02	6.8675E-02	2.9424E-03	*****	*****	*****
17	4.4801E-03	7.1852E-02	2.6718E-01	1.0776E-01	6.3088E-02	2.3488E-02	7.4348E-02	*****	*****	*****
18	1.0894E-04	6.6745E-03	9.2613E-02	2.8246E-01	6.7723E-02	8.7269E-02	6.1701E-03	*****	*****	*****
19	2.1785E-07	1.6584E-04	9.6153E-03	1.1555E-01	2.8900E-01	3.5244E-02	1.0409E-01	*****	*****	*****

SPECTROGRAPHIC CONSTANTS FROM HERZBERG
MORSE FRANCK CONDON FACTORS NBS VOL 65A 1961 P 451.
THIS TRANSITION COMPUTED IN SUBROUTINE ZERO

		ELECTRONIC DECENERGY	ELECTRONIC TERM ENERGY	WE	WEZE	WEYE	WEZE	BE	ALPHA E
UPPER STATE	6	8.91473CGE 04	2.C351000E 03	1.7C80000E 01	-2.1500000E 00	0.0000000E-39	1.82590CGE 00	1.9700000E-02	
LCWER STATE	6	5.9626300E 04	1.7341100E 03	1.4470000E 01	0.0000000E-39	0.0000000E-39	1.6380000E 00	1.8400000E-02	
	1	9.9327000E 04	6.7C000CGE 02	0.C000000E-39	0.C000000E-39	0.C000000E-39	1.46000CGE 00	0.0000000E-39	
	3	9.7584000E 04	0.C0000CGE-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	
	3	9.5774000E 04	2.18450CGE 03	0.C000000E-39	0.C000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	
	2	6.929C000E 04	1.6520100E 03	1.2791000E 01	-3.4890000E-01	0.0000000E-39	1.6370000E 00	2.2400000E-02	
	6	2.9943000E 04	1.5601C00E 03	1.1900000E 01	0.C000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	
	1	6.C00C000E 04	1.52700CGE 03	1.1500000E 01	0.0000000E-39	0.0000000E-39	1.4800000E 00	1.5000000E-02	
	3	5.C2C6000E 04	1.46C37CGE 03	1.3891000E 01	-2.5C00000E-02	0.0000000E-39	1.44000CGE 00	1.3000000E-02	
	1	0.C000000E-39	2.35961CGE 03	1.4456000E 01	7.5100000E-04	-5.9900000E-04	2.0100000E 00	1.87C0000E-02	

[illegible][illegible]

SPECTROGRAPHIC CONSTANTS FROM HERZBERG.
MORSE FRANCK CONDN FACTORS NBS VOL 65A P 451 1961
THIS TRANSITION COMPUTED IN SUBROUTINE ONE.

	LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT		
	2.	1.0	10	7.0038		
	SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT GE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
UPPER STATE	0.00	1	0.0000000E-38	0.0000000E-38	0.0000000E-38	C.1213000E-07
LOWER STATE	0.00	0	0.0000000E-38	0.0000000E-38	0.7871000E 05	C.1094000E-07

		ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEXE	WEYE	WEZE	BE	ALPHA E
UPPER STATE	2	6.9290000E 04	1.6520100E 03	1.2791000E 01	-3.4900000E-01	0.0000000E-39	1.6370000E 00	2.2400000E-02	
LOWER STATE	1	0.0000000E-39	2.3596100E 03	1.4456000E 01	7.5100000E-03	-5.0900000E-04	2.0100000E 00	1.8700000E-02	
	1	5.9327000E 04	6.7000000E C2	0.0000000E-39	0.0000000E-39	0.0000000E-39	1.4600000E 00	0.0000000E-39	
	3	5.7584000E 04	C.0000000E-39	C.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	
	3	5.9770000E 04	2.1845000E 03	0.0000000E-39	C.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	
	6	8.9147300E 04	2.C351000E 03	1.7080000E 01	-2.1500000E 00	0.0000000E-39	1.8259000E 00	1.9700000E-02	
	2	6.3943000E 04	1.5601000E 03	1.1900000E 01	C.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39	
	1	6.C000000E 04	1.5270000E 03	1.1500000E 01	0.0000000E-39	0.0000000E-39	1.4800000E 00	1.5000000E-02	
	6	5.5626300E 04	1.7341100E 03	1.4470000E 01	C.0000000E-39	C.0000000E-39	1.6380000E 00	1.8400000E-02	
	3	5.C2C6000E 04	1.4603700E 03	1.3891000E 01	-2.5000000E-02	0.0000000E-39	1.4400000E 00	1.3000000E-02	

FRANK-CCNCCN FACTOR

[illegible][illegible]

DIATOMIC
TRANSITION
NO 8

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
1

NUMBER
SPECIFYING
DATA LOCATION
ON TAPE
10

SPECTROGRAPHIC CONSTANTS FROM HERZBERG.
AVERAGE VALUES FOR PI 1/2 AND PI 3/2 USED IN APPROPRIATE PLACES.
RRR FRANCK-CONDON FACTORS JQSRT VOL 4 P271 UPPER VALUE IN ARRAY USED
THIS TRANSITION COMPUTED IN SUBROUTINE ZERO.

LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR MONONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT
0.	0.0	6	7.4688

SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT CE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
UPPER STATE 0.00	1	0.0000000E-38	0.0000000E-38	0.0000000E-38	0.1416500E-07
LOWER STATE 124.20	1	0.0000000E-38	0.0000000E-38	0.5240000E 05	0.1150800E-07

ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEZE	WEYE	WEZE	BE	ALPHA E
UPPER STATE 4	4.5922400E 04	1.C376800E 03	7.6C30000E 00	5.6700000E-02	0.0000000E-39	1.1270000E 00	1.5250000E-02
LOWER STATE 4	6.0550000E 01	1.9C38550E 03	1.3970000E 01	-1.2000000E-03	0.0000000E-39	1.7046000E 00	1.7800000E-02
2	6.C628500E 04	2.2736000E 03	1.5850000E 01	0.0000000E-39	0.0000000E-39	1.9863000E 00	1.8200000E-02
2	5.3C83000E 04	2.3270000E 03	2.3C00000E 01	0.0000000E-39	0.0000000E-39	1.9917000E 00	0.0000000E-39
2	5.2148000E 04	2.3470000E 03	0.0C00000E-39	0.0000000E-39	0.0000000E-39	1.9550000E 00	0.0000000E-39
2	4.3965700E 04	2.3713000E 03	1.4480000E 01	-2.8000000E-01	0.0000000E-39	1.9952000E 00	1.6400000E-02

FRANCK-CONDON FACTOR

VV	0	1	2	3	4	5	6	7	8	9
V										
0	*****	*****	1.0000E-C3	5.0000E-03	1.7000E-02	4.1000E-02	8.2000E-02	1.2500E-01	1.6300E-01	1.6700E-01
1	*****	1.0000E-03	6.0000E-C3	2.4000E-02	5.1000E-02	9.7000E-02	1.1700E-01	8.8000E-02	2.9000E-02	*****
2	*****	4.0000E-03	1.8000E-C2	4.8000E-C2	8.5000E-02	9.2000E-02	4.7000E-02	2.0000E-03	2.1000E-C2	7.3000E-C2
3	1.CCC0E-C3	9.0000E-03	3.8000E-02	7.6000E-02	8.4000E-02	3.8000E-02	*****	3.3000E-02	6.8000E-02	4.2000E-02
4	3.0000E-C3	1.7000E-02	5.4000E-C2	7.6000E-02	4.3000E-02	1.0000E-03	3.0000E-02	6.0000E-02	2.1000E-02	3.0000E-03
5	5.0000E-03	3.2000E-02	6.9000E-02	5.7000E-02	6.0000E-03	1.2000E-02	5.3000E-02	2.4000E-02	4.0000E-03	4.6000E-02
6	1.1000E-02	4.4000E-C2	7.0000E-02	3.2000E-02	1.0000E-03	3.8000E-C2	3.5000E-C2	2.4000E-02	3.1000E-02	3.4000E-C2
7	1.7000E-02	5.9000E-02	5.3000E-02	7.0000E-03	2.4000E-02	4.6000E-02	5.0000E-03	2.3000E-02	3.6000E-02	1.0000E-03
8	2.2000E-02	5.8000E-02	3.6000E-C2	*****	3.4000E-02	2.7000E-02	2.0000E-03	3.8000E-02	1.4000E-02	1.0000E-02
9	2.9000E-02	6.0000E-02	1.9000E-C2	1.4000E-02	4.2000E-02	6.0000E-03	1.8000E-02	3.1000E-02	*****	3.0000E-02
10	3.2000E-C2	5.7000E-C2	8.0000E-C3	2.0000E-02	3.4000E-02	*****	3.2000E-02	1.0000E-02	1.4000E-02	2.7000E-02
11	4.1000E-C2	4.8000E-02	1.0000E-C3	3.1000E-02	2.0000E-02	5.0000E-03	3.1000E-02	*****	2.8000E-02	9.0000E-03
12	5.1000E-02	3.4000E-C2	3.0000E-C3	3.8000E-02	1.0000E-03	2.6000E-02	1.1000E-02	1.3000E-02	2.0000E-02	3.0000E-03
13	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
14	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
15	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
16	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
17	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
18	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
19	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

VV	10	11	12	13	14	15	16	17	18	19
V										
0	1.5200E-01	1.1400E-01	7.6000E-C2	3.3000E-02	1.6000E-02	7.0000E-03	2.0000E-03	*****	*****	*****
1	2.1000E-02	7.4000E-02	1.2600E-01	1.3900E-01	1.0500E-01	6.8000E-02	2.8000E-02	1.2000E-02	4.0000E-03	1.0000E-03
2	8.2000E-C2	4.1000E-C2	*****	1.8000E-C2	8.2000E-C2	1.2600E-01	1.2400E-01	7.7000E-02	5.0000E-02	1.0000E-C2
3	1.CCC0E-C3	2.4000E-C2	7.2000E-C2	5.4000E-02	9.0000E-03	1.3000E-02	8.6000E-C2	1.3400E-01	1.1500E-01	6.9000E-02
4	3.9000E-02	5.4000E-C2	1.2000E-02	1.7000E-02	6.6000E-02	5.6000E-02	5.0000E-03	2.9000E-02	7.7000E-02	1.2900E-01
5	3.7000E-02	1.8000E-02	2.5000E-C2	5.2000E-02	1.4000E-02	1.0000E-02	6.3000E-02	5.0000E-02	3.0000E-03	3.0000E-02
6	1.0000E-03	2.5000E-C2	4.3000E-C2	2.0000E-03	1.8000E-02	5.0000E-02	6.0000E-03	1.8000E-02	6.2000E-02	4.0000E-02
7	2.2000E-02	4.0000E-02	2.0000E-C3	2.8000E-02	3.4000E-02	*****	3.1000E-02	4.2000E-02	1.0000E-03	3.8000E-02
8	3.5000E-C2	2.0000E-C3	1.7000E-02	2.7000E-02	*****	3.3000E-02	2.2000E-C2	*****	3.5000E-02	3.2000E-02
9	1.8000E-02	8.0000E-C3	3.4000E-C2	2.0000E-03	2.1000E-02	3.0000E-02	*****	3.2000E-02	2.2000E-02	8.0000E-03
10	*****	2.4000E-C2	1.4000E-C2	1.4000E-02	2.7000E-C2	*****	2.7000E-02	1.4000E-02	3.0000E-03	4.1000E-02
11	8.0000E-C3	2.6000E-C2	*****	3.2000E-02	8.0000E-03	1.8000E-02	2.2000E-02	2.0000E-02	2.6000E-02	6.0000E-03
12	2.6000E-02	1.0000E-03	1.2000E-C2	7.0000E-03	8.0000E-03	2.2000E-C2	1.0000E-03	3.1000E-02	5.0000E-03	2.2000E-02
13	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
14	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
15	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
16	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
17	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
18	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
19	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

DIATOMIC
TRANSITION
NO 6

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
3

NUMBER
SPECIFYING
DATA LOCATION
ON TAPE
11

SPECTROGRAPHIC CONSTANTS FROM HERZBERG
AVERAGE VALUES OF PI 1/2 AND PI 3/2 IN APPROPRIATE PLACES.
RRR FRANCK CONDON FACTORS JQSRT VOL 4 P271 1964
THIS TRANSITION COMPUTED IN SUBROUTINE S2 P12

LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT
0.	0.0	6	7.4688

SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
UPPER STATE C.00	0	0.0000000E-38	0.0000000E-38	0.0000000E-38	0.1063700E-07
LOWER STATE 124.20	1	0.0000000E-38	0.0000000E-38	0.5240000E 05	0.1150800E-07

ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEZE	WEYE	WEZE	BE	ALPHA E
UPPER STATE 2	4.3965700E 04	2.371300CE 03	1.4480000E 01	-2.8000000E-01	0.0000000E-39	1.9952000E 00	1.6400000E-02
LOWER STATE 4	6.0550000E 01	1.9038550E 03	1.3970000E 01	-1.2000000E-03	0.0000000E-39	1.7046000E 00	1.7800000E-02
2	6.0628500E 04	2.373600CE 03	1.5850000E 01	0.0000000E-39	0.0000000E-39	1.5863000E 00	1.8200000E-02
2	5.3083000E 04	2.3270000E 03	2.3000000E 01	0.0000000E-39	0.0000000E-39	1.9917000E 00	0.0000000E-39
2	5.2148000E 04	2.3470000E 03	0.0000000E-39	0.0000000E-39	0.0000000E-39	1.9550000E 00	0.0000000E-39
4	4.5932400E 04	1.0376800E 03	7.6030000E 00	5.6700000E-02	0.0000000E-39	1.1270000E 00	1.5250000E-02

FRANCK-CONDON FACTOR

VV	0	1	2	3	4	5	6	7	8	9	
V	0	2.2700E-01	3.0500E-01	2.1800E-01	1.3300E-01	6.5000E-02	2.8000E-02	1.0000E-02	3.0000E-03	2.0000E-03	1.0000E-03
0	1	3.6700E-01	5.6000E-02	2.4000E-02	1.3300E-01	1.6000E-01	1.2600E-01	7.0000E-02	3.4000E-02	1.3000E-02	6.0000E-03
1	2	2.7500E-01	8.7000E-02	1.6900E-01	1.5000E-02	2.0000E-02	9.2000E-02	1.2500E-01	1.0600E-01	6.1000E-02	2.8000E-02
2	3	9.9000E-02	2.7400E-01	1.0000E-03	1.1200E-01	9.4000E-02	4.0000E-02	2.6000E-02	8.5000E-02	1.0100E-01	8.3000E-02
3	4	2.6000E-02	1.9300E-01	1.7400E-01	5.3000E-02	2.0000E-02	1.0900E-01	5.6000E-02	*****	3.1000E-02	8.3000E-02
4	5	5.0000E-03	7.7000E-02	2.7000E-01	4.8000E-02	6.0000E-03	1.2700E-01	2.2000E-02	2.6000E-02	9.2000E-02	3.6000E-02
5	6	2.0000E-03	1.0000E-02	1.0500E-01	2.3400E-01	1.4900E-01	1.8000E-02	4.9000E-02	7.7000E-02	5.0000E-03	5.5000E-02
6	7	*****	1.0000E-03	3.0000E-02	1.9200E-01	2.2100E-01	5.2000E-02	9.3000E-02	2.5000E-02	9.2000E-02	1.8000E-02
7	8	*****	*****	*****	6.0000E-02	1.1000E-01	2.3000E-01	6.0000E-03	1.0600E-01	3.0000E-03	7.5000E-02
8	9	*****	*****	*****	3.0000E-03	3.0000E-03	2.4000E-02	1.7900E-01	2.0000E-03	9.9000E-02	1.6000E-02
9	10	*****	*****	*****	1.0000E-03	1.3000E-02	9.3000E-02	1.2300E-01	2.6000E-02	8.0000E-02	8.0000E-02
10	11	*****	*****	*****	4.0000E-03	6.1000E-02	1.8600E-01	2.0400E-01	6.2000E-02	6.9000E-02	6.9000E-02
11	12	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
12	13	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
13	14	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
14	15	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
15	16	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
16	17	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
17	18	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
18	19	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

VV	10	11	12	13	14	15	16	17	18	19
V	0	*****	*****	*****	*****	*****	*****	*****	*****	*****
0	1	3.0000E-03	1.0000E-03	*****	*****	*****	*****	*****	*****	*****
1	2	1.4000E-02	7.0000E-03	4.0000E-03	2.0000E-03	1.0000E-03	*****	*****	*****	*****
2	3	6.0000E-02	3.3000E-02	1.4000E-02	7.0000E-03	3.0000E-03	*****	*****	*****	*****
3	4	8.5000E-02	6.7000E-02	4.0000E-02	3.2000E-02	1.4000E-02	7.0000E-03	1.0000E-03	*****	*****
4	5	2.5000E-02	7.1000E-02	7.5000E-02	5.9000E-02	3.8000E-02	2.4000E-02	1.8000E-02	6.0000E-03	2.0000E-03
5	6	*****	1.7000E-02	6.5000E-02	7.4000E-02	6.5000E-02	5.6000E-02	5.4000E-02	2.8000E-02	2.4000E-02
6	7	6.8000E-02	3.0000E-02	*****	2.0000E-02	6.1000E-02	7.1000E-02	5.2000E-02	5.6000E-02	3.4000E-02
7	8	1.1000E-02	5.9000E-02	1.7000E-02	4.1000E-02	2.1000E-02	1.3000E-02	6.2000E-02	5.4000E-02	5.3000E-02
8	9	3.4000E-02	3.0000E-03	4.1000E-02	5.3000E-02	2.0000E-02	8.0000E-03	4.0000E-03	3.4000E-02	4.6000E-02
9	10	5.3000E-02	6.3000E-02	2.0000E-03	1.4000E-02	5.0000E-02	3.4000E-02	1.2000E-02	*****	1.0000E-02
10	11	2.5000E-02	2.4000E-02	6.5000E-02	3.2000E-02	9.0000E-03	3.5000E-02	4.8000E-02	2.4000E-02	1.3000E-02
11	12	4.5000E-02	5.5000E-02	2.0000E-03	5.4000E-02	2.9000E-02	3.0000E-03	1.4000E-02	3.2000E-02	*****
12	13	*****	*****	*****	*****	*****	*****	*****	*****	*****
13	14	*****	*****	*****	*****	*****	*****	*****	*****	*****
14	15	*****	*****	*****	*****	*****	*****	*****	*****	*****
15	16	*****	*****	*****	*****	*****	*****	*****	*****	*****
16	17	*****	*****	*****	*****	*****	*****	*****	*****	*****
17	18	*****	*****	*****	*****	*****	*****	*****	*****	*****
18	19	*****	*****	*****	*****	*****	*****	*****	*****	*****

DIATOMIC
TRANSITION
COASDI

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
2

NUMBER
SPECIFYING
DATA LOCATION
ON TAPE
12

COASDI STANDS FOR CO ASLNDI BANDS.
SPECTROGRAPHIC CONSTANTS FROM HERZBERG.
MORSE FRANK-CONDON FACTORS BY JARMAIN, FRASER, AND NICHOLLS
ASTROPHYS J 122,55, (1955)
THIS TRANSITION COMPUTED IN SUBROUTINE ONE.

LINE ALTERNATION FACTOR		NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES		NUMBER OF ELECTRONIC LEVELS		REDUCED ATOMIC WEIGHT	
C.		0.0		12		6.8584	
UPPER STATE	C.00	0	0.0000000E-38	C.0000000E-38	C.0000000E-38	C.0000000E-38	0.1359000E-07
LOWER STATE	0.00	1	0.0000000E-38	0.0000000E-38	0.0000000E-38	0.0000000E-38	C.1209300E-07

SPIN COUPLING CONSTANT		QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS		ROTATIONAL CONSTANT DE, 1/CM		ROTATIONAL CONSTANT BETA, 1/CM		DISSOCIATION ENERGY DEFFRO, 1/CM		INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM	
UPPER STATE	3	5.591000E 04	1.218000E 03	9.500000E 00	0.000000E-39	0.000000E-39	0.000000E-39	1.331000E 00	1.600000E-02		
LOWER STATE	6	4.8687550E 04	1.7392500E 03	1.447000E 01	0.000000E-39	0.000000E-39	0.000000E-39	1.681000E 00	1.930000E-02		

ELECTRONIC DEGENERACY		ELECTRONIC TERM ENERGY		WE		WEEXE		WEYE		WEZE		BE		ALPHA E	
UPPER STATE	3	5.591000E 04	1.218000E 03	9.500000E 00	0.000000E-39	0.000000E-39	0.000000E-39	0.000000E-39	0.000000E-39	0.000000E-39	0.000000E-39	1.331000E 00	1.600000E-02		
LOWER STATE	6	4.8687550E 04	1.7392500E 03	1.447000E 01	0.000000E-39	0.000000E-39	0.000000E-39	0.000000E-39	0.000000E-39	0.000000E-39	0.000000E-39	1.681000E 00	1.930000E-02		

FRANK-CONDON FACTOR

VV	C	1	2	3	4	5	6	7	8	9
0	3.7000E-02	1.4300E-01	2.4300E-01	*****	*****	*****	*****	*****	*****	*****
1	1.0300E-01	1.9500E-01	9.7000E-02	*****	*****	*****	*****	*****	*****	*****
2	1.6200E-01	1.0500E-01	*****	*****	*****	*****	*****	*****	*****	*****
3	1.8100E-01	1.9000E-02	5.0000E-02	*****	*****	*****	*****	*****	*****	*****
4	1.6500E-01	3.0000E-03	5.5000E-02	*****	*****	*****	*****	*****	*****	*****
5	1.2900E-01	3.9000E-02	6.7000E-02	*****	*****	*****	*****	*****	*****	*****
6	5.1000E-02	8.1000E-02	2.4000E-02	*****	*****	*****	*****	*****	*****	*****
7	5.9000E-02	1.0200E-01	1.0000E-03	*****	*****	*****	*****	*****	*****	*****
8	3.6000E-02	9.9000E-02	5.0000E-03	*****	*****	*****	*****	*****	*****	*****
9	2.1000E-02	8.2000E-02	2.3000E-02	*****	*****	*****	*****	*****	*****	*****
10	1.9000E-02	6.4000E-02	4.1000E-02	*****	*****	*****	*****	*****	*****	*****
11	1.2000E-02	5.0000E-02	5.2000E-02	*****	*****	*****	*****	*****	*****	*****
12	7.0000E-03	3.8000E-02	5.5000E-02	*****	*****	*****	*****	*****	*****	*****
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VV	1C	11	12	13	14	15	16	17	18	19
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DIATOMIC
TRANSITION
C2PHIL

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
2

NUMBER
SPECIFYING
DATA LOCATION
ON TAPE
13

C2PHIL STANDS FOR C2 PHILLIPS BANDS.
SPECTROGRAPHIC CONSTANTS FROM BALLIK AND RAMSAY ASTROPHYS J 137 1963 P84.
RRR FRANCK-CONDON FACTORS JQSRT VOL 5 1965 P 165.
TRANSITION COMPUTED IN SUBROUTINE CNE.

LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT
2.	0.0	10	6.0019

SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
UPPER STATE C.00	1	0.0000000E-38	C.0000000E-38	0.4130000E C5	C.1318430E-07
LOWER STATE 0.00	0	0.0000000E-38	C.0000000E-38	0.4960000E 05	0.1242530E-07

ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WE XE	WE YE	WE ZE	BE	ALPHA E
UPPER STATE 2	8.391000E 03	1.6083500E 03	1.2078000E 01	-1.0000000E-02	0.0000000E-39	1.616340E 00	1.6880000E-02
LOWER STATE 1	0.0000000E-39	1.8547100E 03	1.3340000E 01	-1.7200000E-01	0.0000000E-39	1.8198400E 00	1.7650000E-02
1	5.5024600E 04	1.6715000E 03	4.0020000E 01	2.4600000E-01	0.0000000E-39	1.7920000E 00	4.2100000E-02
1	4.3240230E 04	1.8295700E 03	1.3970000E 01	0.0000000E-39	0.0000000E-39	1.8334000E 00	2.0400000E-02
6	4.0796650E 04	1.1065600E 03	3.5260000E 01	2.8500000E 00	0.0000000E-39	1.1922000E 00	2.4200000E-02
2	3.4261900E 04	1.8091000E 03	1.5810000E 01	-4.0200000E 00	0.0000000E-39	1.7834000E 00	1.8000000E-02
6	2.0022500E 04	1.7882200E 03	1.6440000E 01	0.0000000E-39	0.0000000E-39	1.7527000E 00	1.6080000E-02
3	1.3312100E 04	1.5616000E 03	1.3850000E 01	0.0000000E-39	0.0000000E-39	1.8700000E 00	0.0000000E-39
3	6.4342700E 03	1.4704500E 03	1.1190000E 01	2.0000000E-02	0.0000000E-39	1.4985200E 00	1.6340000E-02
6	7.1624000E 02	1.6413500E 03	1.1670000E 01	0.0000000E-39	0.0000000E-39	1.6324600E 00	1.6610000E-02

FRANCK-CONDON FACTOR

VV	0	1	2	3	4	5	6	7	8	9
V										
0	4.1570E-C1	3.9700E-C1	1.5360E-01	3.0200E-02	3.2000E-03	2.0000E-04	*****	*****	*****	*****
1	3.3580E-C1	7.2000E-03	2.9490E-C1	2.6170E-01	8.4800E-02	1.4100E-02	1.4000E-03	2.0000E-04	*****	*****
2	1.5910E-01	1.7800E-C1	5.3000E-C2	1.2380E-01	2.9440E-C1	1.4950E-01	3.5300E-02	5.6000E-03	1.0000E-03	2.0000E-04
3	5.8900E-02	1.9520E-C1	3.5200E-C2	1.4430E-01	1.6700E-02	2.4820E-01	2.0630E-01	7.3100E-02	1.7700E-02	3.6000E-03
4	2.0100E-02	1.2160E-01	1.3570E-C1	1.0000E-03	1.6310E-01	7.4000E-03	1.4430E-01	2.3470E-01	1.2350E-01	3.8300E-C2
5	6.8000E-03	6.0200E-02	1.4290E-C1	5.7200E-02	3.8600E-C2	1.1550E-01	6.6000E-02	4.6800E-02	2.1310E-01	1.6580E-01
6	2.3000E-C3	2.5600E-C2	9.5600E-C2	1.1860E-01	7.8000E-03	8.7500E-02	4.4900E-02	1.2680E-01	2.0000E-03	1.5560E-01
7	8.0000E-04	1.0000E-02	5.1200E-02	1.1350E-01	7.1400E-02	2.5000E-03	1.1480E-01	2.3000E-03	1.4570E-01	1.1800E-02
8	3.0000E-C4	3.6000E-C3	2.3500E-C2	7.6700E-02	1.0850E-C1	2.9100E-02	2.8700E-02	9.9000E-C2	1.0400E-02	1.2020E-01
9	1.0000E-04	1.2000E-03	9.6000E-03	4.2300E-02	9.6600E-02	8.6400E-02	4.7000E-03	6.4600E-02	5.9000E-02	4.5300E-02
10	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
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VV	10	11	12	13	14	15	16	17	18	19
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3	7.0000E-04	*****	*****	*****	*****	*****	*****	*****	*****	*****
4	8.9000E-03	*****	*****	*****	*****	*****	*****	*****	*****	*****
5	6.6000E-02	*****	*****	*****	*****	*****	*****	*****	*****	*****
6	1.9520E-01	*****	*****	*****	*****	*****	*****	*****	*****	*****
7	5.0600E-02	*****	*****	*****	*****	*****	*****	*****	*****	*****
8	5.0100E-02	*****	*****	*****	*****	*****	*****	*****	*****	*****
9	7.5700E-02	*****	*****	*****	*****	*****	*****	*****	*****	*****
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DIATOMIC
TRANSITION
Q2 SR

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
1

NUMBER
SPECIFYING
DATA LOCATION
ON TAPE
14

SPECTROGRAPHIC CONSTANTS FROM FERZBERG.
MORSE FRANCK-CONDON FACTORS BY JARMAIN, FRASER, AND NICHOLLS 1954
ASTROPHYS J 122, 55 (1955)
TRANSITION COMPUTED IN SUBROUTINE ZERO.

LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR MONONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT
1.	0.0	5	8.0000

SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
UPPER STATE C.00	C	0.0000000E-38	C.0000000E-38	0.1430000E 05	C.16C4C00E-07
LOWER STATE C.00	C	0.0000000E-38	C.0000000E-38	0.4760000E 05	0.1207398E-07

ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEKE	WEYE	WEZE	BE	ALPHA E
UPPER STATE 3	4.58C21CCE 04	7.0C36CCCE 02	8.00230CCE 00	-3.753500CE-C1	0.0000000E-39	8.19C00CCE-C1	1.10C0000E-02
LOWER STATE 3	0.0000000E-39	1.5803610E 03	1.2073000E 01	5.4600000E-02	-1.4300000E-03	1.4456660E 00	1.5791000E-02
3	3.6C960CCE 04	8.1500000E 02	2.2500CCE 01	C.0000000E-39	C.0000000E-39	1.05000CCE 00	0.0000000E-39
1	1.3195220E 04	1.4326870E 03	1.395008CE 01	-1.0750000E-02	0.0000000E-39	1.4004160E 00	1.8170000E-02
2	7.91810CCE 03	1.5C93CCCE 03	1.29000CCE 01	C.0000000E-39	0.0000000E-39	1.42640CCE 00	1.7100000E-02

FRANCK-CONDON FACTOR

VV	C	1	2	3	4	5	6	7	8	9
V										
0	2.3100E-09	6.2500E-08	8.1200E-07	*****	*****	*****	*****	*****	*****	*****
1	2.6500E-08	6.6400E-07	7.8400E-06	*****	*****	*****	*****	*****	*****	*****
2	1.6400E-07	3.6900E-06	5.6100E-05	*****	*****	*****	*****	*****	*****	*****
3	6.5400E-07	1.4300E-05	1.3500E-04	*****	*****	*****	*****	*****	*****	*****
4	2.2800E-06	4.3200E-05	3.8000E-04	*****	*****	*****	*****	*****	*****	*****
5	6.3000E-06	8.4800E-05	8.6400E-04	*****	*****	*****	*****	*****	*****	*****
6	1.5000E-05	2.3700E-04	1.7100E-03	*****	*****	*****	*****	*****	*****	*****
7	3.1800E-05	4.6200E-04	3.0000E-03	*****	*****	*****	*****	*****	*****	*****
8	6.1200E-05	8.1200E-04	4.8000E-02	*****	*****	*****	*****	*****	*****	*****
9	1.0800E-04	1.3200E-03	7.0700E-03	*****	*****	*****	*****	*****	*****	*****
10	1.8000E-04	2.0200E-03	9.7200E-03	*****	*****	*****	*****	*****	*****	*****
11	2.7900E-04	2.8500E-03	1.2500E-02	*****	*****	*****	*****	*****	*****	*****
12	4.1600E-04	3.9400E-03	1.5400E-02	*****	*****	*****	*****	*****	*****	*****
13	5.8800E-04	5.1300E-03	1.8200E-02	*****	*****	*****	*****	*****	*****	*****
14	7.5500E-04	6.4200E-03	2.0400E-02	*****	*****	*****	*****	*****	*****	*****
15	1.0400E-03	7.7400E-03	2.2200E-02	*****	*****	*****	*****	*****	*****	*****
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VV	1C	11	12	13	14	15	16	17	18	19
V										
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DIATOMIC
TRANSITION
CH4300

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
2

NUMBER
SPECIFYING
DATA LOCATION
CN TAPE
15

SPECTROGRAPHIC CONSTANTS FROM HERZBERG.
MORSE FRANK-CONDON FACTORS JQSRT VOL 4 P283 1964
TRANSITION COMPUTED IN SUBROUTINE CNE.

	LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT
	C.	0.0	4	C.9300

	SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY CEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
UPPER STATE	0.00	2	0.0000000E-38	0.0000000E-38	0.0000000E-38	C.1102600E-07
LOWER STATE	0.00	1	0.0000000E-38	0.0000000E-38	0.2800000E 05	0.1119800E-07

	ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEZE	WEYE	WEZE	BE	ALPHA E
UPPER STATE	4	2.3150000E 04	2.9210000E 03	9.0400000E 01	0.0000000E-39	0.0000000E-39	1.4912000E 01	6.7000000E-01
LOWER STATE	4	0.0000000E-39	2.8616000E 03	6.4300000E 01	0.0000000E-39	0.0000000E-39	1.4457000E 01	5.3400000E-01
	2	3.1821000E 04	2.8241000E 03	1.0580000E 02	0.0000000E-39	0.0000000E-39	1.4629000E 01	7.4400000E-01
	2	2.5949000E 04	2.5425000E 03	3.7380000E 02	0.0000000E-39	0.0000000E-39	1.2887000E 01	4.8500000E-01

FRANK-CONDON FACTOR

VV	C	1	2	3	4	5	6	7	8	9
V										
0	9.9960E-01	2.0000E-04	*****	*****	*****	*****	*****	*****	*****	*****
1	2.0000E-04	9.9860E-01	1.0000E-04	*****	1.0000E-04	*****	*****	*****	*****	*****
2	*****	1.0000E-04	9.5470E-01	2.8000E-03	*****	*****	*****	*****	*****	*****
3	*****	*****	3.2000E-03	9.8150E-01	1.3100E-02	1.6000E-03	1.0000E-04	*****	*****	*****
4	*****	*****	*****	1.4600E-02	9.2530E-01	4.2100E-02	*****	*****	*****	*****
5	*****	*****	*****	*****	4.9600E-02	8.8620E-01	*****	*****	*****	*****
6	*****	*****	1.0000E-04	2.3000E-03	1.2800E-02	*****	*****	*****	*****	*****
7	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
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VV	10	11	12	13	14	15	16	17	18	19
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DIATOMIC
TRANSITION
CH3500

INDEX NO.
SPECIFYING
SUBROUTINE
USED IN CALC.
3

NUMBER
SPECIFYING
DATA LOCATION
ON TAPE
16

SPECTROGRAPHIC CONSTANTS FROM HERZBERG
MORSE FRANCK-CONDON FACTORS JQSRT VOL 4 P283 1964
TRANSITION COMPUTED IN SUBROUTINE S2 P12.

LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR MONONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT	SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
0.	0.0	4	C.9300						
UPPER STATE	0.00	C				C.0000000E-38	C.0000000E-38	C.0000000E-38	C.11861CCE-07
LOWER STATE	27.95	1				0.0000000E-38	0.0000000E-38	0.2800000E 05	0.1119800E-07

	ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEZE	WEYE	WEZE	BE	ALPHA E
UPPER STATE	2	2.5949000E 04	2.54250CCE 03	3.7380000E 02	C.0000000E-39	C.0000000E-39	1.2887000E 01	4.8500000E-01
LOWER STATE	4	0.0000000E-39	2.8616000E 03	6.4300000E 01	0.0000000E-39	C.0000000E-39	1.4457000E 01	5.3400000E-01
	2	3.18210CCE 04	2.8241CCE 03	1.0580000E 02	C.0000000E-39	C.0000000E-39	1.4629000E 01	7.4400000E-01
	4	2.3150000E 04	2.9210000E 03	9.0400000E 01	C.0000000E-39	0.0000000E-39	1.4912000E 01	6.7000000E-01

FRANCK-CONDON FACTOR

VV	0	1	2	3	4	5	6	7	8	9
V										
0	5.9370E-01	6.0000E-04	1.6910E-01	5.2500E-02	8.0000E-03	5.5700E-02	3.3100E-02	1.7000E-03	*****	*****
1	1.3000E-03	2.1760E-01	1.6700E-02	1.1160E-01	1.3970E-01	6.8000E-03	4.5700E-02	1.1270E-01	*****	*****
2	1.8450E-01	1.6600E-02	4.0000E-04	1.6200E-02	1.8000E-03	4.5300E-02	2.4400E-02	6.0000E-04	*****	*****
3	*****	2.1740E-01	1.2000E-03	7.4500E-02	8.7000E-03	9.2000E-03	4.2800E-02	7.9100E-02	*****	*****
4	8.1100E-02	1.6500E-02	5.7600E-02	1.4200E-02	3.8900E-02	4.9000E-03	3.9000E-03	*****	*****	*****
5	7.0000E-04	1.6100E-01	2.1500E-02	1.0000E-03	*****	*****	*****	*****	*****	*****
6	3.8300E-02	1.0200E-02	8.1300E-02	5.1300E-02	*****	*****	*****	*****	*****	*****
7	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
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VV	10	11	12	13	14	15	16	17	18	19
V										
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19	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****

DIATOMIC TRANSITION BE0B-X INDEX NO. SPECIFYING SUBROUTINE USED IN CALC. 1 NUMBER SPECIFYING DATA LOCATION ON TAPE 17

SPECTROGRAPHIC CONSTANTS FROM HERZBERG.
MORSE FRANK CONDON FACTORS JQSRT VOL 7 P639 1967.
VALUES USED WERE THE AVERAGE OF THOSE FOR THE P AND R BRANCHES FOR J=20.
THIS TRANSITION COMPUTED IN SUBROUTINE ZERO.

LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT
0.	0.0	5	5.7661

SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS	ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
UPPER STATE 0.00	C	0.0000000E-38	0.0000000E-38	0.0000000E-38	0.1362200E-07
LOWER STATE 0.00	0	0.0000000E-38	0.0000000E-38	0.2990000E 05	0.1330800E-07

ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEWE	WEYE	WEZE	BE	ALPHA E
UPPER STATE 1	2.1253940E 04	1.3708170E 03	7.7455000E 00	-2.7000000E-04	0.0000000E-39	1.5758000E 00	1.5400000E-02
LOWER STATE 1	0.0000000E-39	1.4873230E 03	1.1825700E 01	2.2350000E-02	0.0000000E-39	1.6510000E 00	1.9000000E-02
2	4.1365000E 04	1.6160000E 03	1.0000000E 01	0.0000000E-39	0.0000000E-39	0.0000000E-39	0.0000000E-39
1	3.9126100E 04	1.0815000E 03	9.0000000E 00	0.0000000E-39	0.0000000E-39	1.3080000E 00	1.0000000E-02
2	9.4056100E 03	1.1442380E 03	8.4145000E 00	3.3890000E-02	0.0000000E-39	1.3661000E 00	1.6280000E-02

FRANK-CONDON FACTOR

VV	0	1	2	3	4	5	6	7	8	9
V										
0	8.9250E-01	1.0450E-01	4.1500E-03	*****	*****	*****	*****	*****	*****	*****
1	1.0085E-01	7.0975E-01	1.8030E-01	1.0200E-02	*****	*****	*****	*****	*****	*****
2	7.4500E-03	1.6650E-01	5.7450E-01	2.3545E-01	1.6850E-02	*****	*****	*****	*****	*****
3	*****	1.8750E-02	2.0825E-01	4.7480E-01	2.7600E-01	*****	*****	*****	*****	*****
4	*****	*****	3.1550E-02	2.3210E-01	4.0220E-01	*****	*****	*****	*****	*****
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VV	10	11	12	13	14	15	16	17	18	19
V										
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DIATOMIC TRANSITION CO+ CT INDEX NO. SPECIFYING SUBROUTINE USED IN CALC. 3 NUMBER SPECIFYING DATA LOCATION ON TAPE 18

SPECTROSCOPIC CONSTANTS FROM HERZBERG.
MORSE FRANK-CONDON FACTORS BY JARMAIN, FRASER, AND NICHOLLS 1954
ASTROPHYS J 122, 55 (1955)
THIS TRANSITION COMPUTED IN SUBROUTINE S2 P12.

LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES	NUMBER OF ELECTRONIC LEVELS	REDUCED ATOMIC WEIGHT
0.	0.0	3	6.8582

SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUCL. AXIS	ROTATIONAL CONSTANT CE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM
UPPER STATE 125.00	1	0.0000000E-38	0.0000000E-38	0.0000000E-38	C.1243680E-C7
LOWER STATE 0.00	0	0.0000000E-38	0.0000000E-38	0.7990000E 05	0.1115060E-07

ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEZE	WEYE	WEZE	BE	ALPHA E
UPPER STATE 4	2.0733190E 04	1.5620600E 03	1.3532000E 01	1.3100000E-02	0.0000000E-39	1.5894000E 00	1.9420000E-02
LOWER STATE 2	0.0000000E-39	2.2142400E 03	1.5164000E 01	-7.0000000E-04	0.0000000E-39	1.9772000E 00	1.8960000E-02
2	4.5876700E 04	1.7341800E 03	2.7927000E 01	3.2830000E-01	0.0000000E-39	1.7959200E 00	3.0250000E-02

FRANK-CONDON FACTOR

VV	0	1	2	3	4	5	6	7	8	9
V										
0	4.2000E-02	1.4900E-C1	2.4600E-C1	2.4900E-01	1.7400E-01	8.9000E-02	3.5000E-02	1.1000E-02	*****	*****
1	1.1300E-C1	1.9100E-01	8.3000E-C2	*****	8.4000E-02	1.8300E-01	1.8000E-01	*****	*****	*****
2	1.6600E-C1	9.9000E-C2	2.0000E-C3	1.0400E-01	8.9000E-02	1.0000E-03	*****	*****	*****	*****
3	1.8000E-01	1.5000E-02	7.1000E-02	7.2000E-02	2.0000E-C3	*****	*****	*****	*****	*****
4	1.5900E-01	4.0000E-03	9.6000E-02	1.0000E-03	*****	*****	*****	*****	*****	*****
5	1.2200E-01	4.1000E-02	5.1000E-C2	*****	*****	*****	*****	*****	*****	*****
6	8.5000E-02	7.8000E-02	*****	*****	*****	*****	*****	*****	*****	*****
7	5.5000E-02	*****	*****	*****	*****	*****	*****	*****	*****	*****
8	2.4000E-C2	*****	*****	*****	*****	*****	*****	*****	*****	*****
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VV	10	11	12	13	14	15	16	17	18	19
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APPENDIX E

SAMPLE CASE

SAMPLE CASE FOR NASA TN
CALCULATION INCLUDES THE (0,0) BAND OF THE CN RED SYSTEM,
2 ATOMIC NITROGEN LINES AND AN INSTRUMENT CALIBRATION.

THE SPECTRUM COMPUTED FROM 10860.00 TO 11085.00 ANGSTROMS AT 0.025 ANGSTROM INTERVALS

CN RED

		TOTAL NUMBER OF MOLECULES PER CC	ELECTRONIC TEMPERATURE DEGREES K		VIBRATIONAL TEMPERATURE DEGREES K		ROTATIONAL TEMPERATURE DEGREES K		
		1.0000E 15	6.0000E 03		6.0000E 03		6.0000E 03		
		LINE ALTERNATION FACTOR	NUCLEAR SPIN FOR HOMONUCLEAR MOLECULES		NUMBER OF ELECTRONIC LEVELS		REDUCED ATOMIC WEIGHT		
		0.	0.0		3		6.4643		
		SPIN COUPLING CONSTANT	QUANTUM NUMBER OF RESULTANT ELECTRONIC ANGULAR MOMENTUM ABOUT INTERNUC. AXIS		ROTATIONAL CONSTANT DE, 1/CM	ROTATIONAL CONSTANT BETA, 1/CM	DISSOCIATION ENERGY DEZERO, 1/CM	INTERNUCLEAR DISTANCE AT EQUILIBRIUM POSITION, CM	
UPPER STATE	-52.20	1			0.5932700E-05	-0.4246000E-07	0.5740000E 05	0.1233200E-07	
LOWER STATE	0.00	0			0.6392000E-05	-0.9570000E-08	0.6680000E 05	0.1171900E-07	
		ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	WE	WEKE	WEYE	WEZE	BE	
UPPER STATE	4	9.2453440E 03	1.8125550E 03	1.2608600E 01	-1.1800000E-02	0.0000000E-39	1.7151000E 00	1.7075700E-02	
LOWER STATE	2	0.0000000E-39	2.0687448E 03	1.3134000E 01	-5.5000000E-03	0.0000000E-39	1.8992000E 00	1.7013300E-02	
	2	2.5751800E 04	2.1686140E 03	2.0200000E 01	0.0000000E-39	0.0000000E-39	1.9701000E 00	2.2150000E-02	
VIBRATIONAL QUANTUM NO. UPPER LOWER	FRANCK- CONDON FACTOR	TRANSITION MOMENT AVERAGED OVER THE ELECTRONIC BAND	ROTATIONAL LINE WIDTH AT HALF-HEIGHT GAUSS LORENTZ VOIGT		RANGE IN LINE WIDTHS	BAND ORIGIN IN ANGSTROMS	ROTATIONAL QUANTUM NUMBERS MIN MAX		INTEGRATED INTENSITY W/CM2-SR
0	0	5.0015E-01	5.2100E-01	0.1200 0.1440 0.2119	5	10968.064	2 150		
									P2 BRANCH 9.0922E-04
									R1 BRANCH 4.5949E-03
									SR21 BRANCH 6.5940E-04
									QP12 BRANCH 7.6646E-05
									Q2 AND QP21 BRANCHES 4.8071E-03
									Q1 AND QR12 BRANCHES 4.3989E-03
									R2 AND RQ21 BRANCHES 5.9004E-03
									P1 AND PQ12 BRANCHES 1.0214E-03
									BAND TOTAL 2.2368E-02
									APPROXIMATE BAND TOTAL 1.0518E-01
									SYSTEM TOTAL 2.2368E-02

ATOMIC LINE SPECTRUM FOR N

		NUMBER OF ATOMS PER CC	ELECTRONIC TEMPERATURE	PARTITION FUNCTION				
		2.0000E 21	6.0000E 03	4.1100E 00				
WAVELENGTH IN ANGSTROMS	ELECTRONIC DEGENERACY	ELECTRONIC TERM ENERGY	EINSTEIN A COEFF	ATOMIC LINE WIDTH AT HALF-HEIGHT GAUSS LORENTZ VOIGT			RANGE IN LINE WIDTHS	INTEGRATED INTENSITY W/CM2-SR
19879.200	6	1.04684E 05	1.6000E 05	0.161	0.194	0.285	5	8.4997E-05
19884.600	8	1.04718E 05	1.4100E 05	0.161	0.194	0.285	5	9.9012E-05
SUM OF THE N							ATOMIC LINES INCLUDED	1.8401E-04
TOTAL OF ALL INTEGRATED INTENSITIES							2.2552E-02	

THIS IS A RADIATIVE TRANSPORT SOLUTION, DEPTH OF ABOVE RADIATING LAYER IS 1.000 CM.

TABULATION OF COMPUTED SPECTRUM

WAVELENGTH ANGSTROMS	INTENSITY W/CM2-MICRON-SR	WAVELENGTH ANGSTROMS	INTENSITY W/CM2-MICRON-SR	WAVELENGTH ANGSTROMS	INTENSITY W/CM2-MICRON-SR	WAVELENGTH ANGSTROMS	INTENSITY W/CM2-MICRON-SR
10860.00	0.0000E-39	10916.26	1.5053E-02	10972.51	5.7327E-02	11028.77	1.4343E-03
10860.02	0.0000E-39	10916.28	1.6037E-02	10972.54	5.9158E-02	11028.79	1.5182E-03
10860.05	0.0000E-39	10916.31	1.7227E-02	10972.56	4.8218E-02	11028.82	1.6098E-03
10860.07	0.0000E-39	10916.33	1.8684E-02	10972.59	5.1178E-02	11028.84	1.7014E-03
10860.10	0.0000E-39	10916.36	2.0432E-02	10972.61	5.4436E-02	11028.87	1.8158E-03
10860.13	0.0000E-39	10916.38	2.2560E-02	10972.64	5.8022E-02	11028.89	1.9379E-03
10860.15	0.0000E-39	10916.41	2.5146E-02	10972.66	6.1974E-02	11028.92	2.0599E-03
10860.17	0.0000E-39	10916.43	2.8328E-02	10972.69	6.6345E-02	11028.94	2.2049E-03
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10916.06	1.2314E-02	10972.31	2.1942E-02	11028.57	1.9821E-02	11084.82	4.0046E 00
10916.08	1.2253E-02	10972.34	5.0835E-02	11028.59	1.9791E-02	11084.85	3.0224E 00
10916.11	1.2299E-02	10972.36	5.1147E-02	11028.62	1.8875E-02	11084.87	2.3066E 00
10916.13	1.2459E-02	10972.39	5.1643E-02	11028.64	1.8044E-02	11084.90	1.7938E 00
10916.16	1.2711E-02	10972.41	5.2353E-02	11028.67	1.7273E-02	11084.92	1.3880E 00
10916.18	1.3092E-02	10972.44	5.3261E-02	11028.69	1.6571E-02	11084.95	1.1321E 00
10916.21	1.3603E-02	10972.46	5.4390E-02	11028.72	1.5930E-02	11084.97	9.4532E-01
10916.23	1.4244E-02	10972.49	5.5740E-02	11028.74	1.3580E-03	11085.00	8.0477E-01

DETECTOR OUTPUT SIGNAL GIVEN BY A SPECIFIED INSTRUMENT RESPONSE

SPECTROGRAPH OR SCANNING SPECTROMETER 1
SPECTRAL RANGE FROM 10865.50 TO 11079.50 ANGSTROMS COMPUTED AT 0.250 ANGSTROM INTERVALS

SLIT FUNCTION SPECIFIED BY LINEAR SEGMENTS

WAVELENGTH ANGSTROMS	SLIT FUNCTION
-2.500	0.0000E-39
-2.250	5.0000E-33
-2.000	2.3100E-02
-1.875	4.2200E-02
-1.750	7.2300E-02
-1.650	1.1040E-01
-1.500	2.5100E-01
-0.850	9.0330E-01
-0.800	9.3370E-01
-0.750	9.4580E-01
-0.700	9.5380E-01
-0.650	9.5980E-01
0.500	9.9600E-01
0.550	1.0000E 00
0.600	9.9600E-01
0.650	9.9400E-01
0.700	9.8890E-01
0.750	9.7890E-01
0.800	9.6380E-01
1.550	2.0080E-01
1.600	1.6360E-01
1.650	1.3550E-01
1.750	9.3400E-02
1.850	6.8300E-02
2.000	4.0200E-02
2.150	1.9130E-02
2.250	1.2000E-02
2.500	0.0000E-39

CENTER OF SLIT FUNCTION ANGSTROMS	COMPUTED SLIT WIDTH ANGSTROMS
0.000	2.5250E 00

SPECTRAL CALIBRATION OF INSTRUMENT THAT MULTIPLIES SLIT FUNCTION TO YIELD INSTRUMENT SENSITIVITY

WAVELENGTH ANGSTROMS	CALIBRATION FUNCTION
10860.000	9.0000E-01
10870.000	8.9000E-01
10880.000	8.8000E-01
10890.000	8.7100E-01
10900.000	8.6000E-01
10910.000	8.4800E-01
10920.000	8.3500E-01
10930.000	8.2200E-01
10940.000	8.1400E-01
10950.000	8.0800E-01
10960.000	7.9500E-01
10970.000	7.8000E-01
10975.000	7.6500E-01
10980.000	7.5000E-01
10990.000	7.3000E-01
11002.000	7.0200E-01
11012.000	6.6500E-01
11018.000	6.5500E-01
11025.000	6.5500E-01
11040.000	6.2000E-01
11062.000	5.5200E-01
11065.000	5.5200E-01
11072.000	5.3500E-01
11080.000	5.2000E-01
11085.000	5.0000E-01

LOCATION OF SLIT CENTER ANGSTROMS	INSTRUMENT OUTPUT (W/CW2-MICRON-SR)* (SENSITIVITY UNITS)
10865.500	0.0000E-39
10865.750	0.0000E-39
10866.000	0.0000E-39
10866.250	0.0000E-39
10866.500	0.0000E-39
10866.750	0.0000E-39
10867.000	0.0000E-39
10867.250	0.0000E-39
.	.
.	.
.	.
.	.
11077.750	4.1266E-01
11078.000	3.7107E-01
11078.250	2.8352E-01
11078.500	1.8575E-01
11078.750	9.6976E-02
11079.000	5.1767E-02
11079.250	5.0561E-02
11079.500	8.4439E-02

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TABLE I. - CONSTANTS FOR $2\Pi \leftrightarrow 2\Sigma$ TRANSITIONS

Branch		Strength equation	SIGNU1	SIGNU2	SIGNS1	SIGNS2	SIGNS3	CONST1	CONST2	CONST3
$2\Pi \rightarrow 2\Sigma$	$2\Sigma \rightarrow 2\Pi$									
P ₂	R ₂	S ₁	+1	+1	+1	-1		+1	+1	
R ₁	P ₁	S ₁	-1	-1	+1	-1		+1	0	
S _{R21}	S _{R21}	S ₁	+1	-1	-1	-1		+1	0/+1	
O _{P12}	O _{P12}	S ₁	-1	+1	-1	-1		+1	+1/0	
Q ₂	Q ₂	S ₂	+1	+1	-1		-1			+1
Q _{P21}	Q _{R12}	S ₁	(same NUBAR as Q ₂)		-1	+1		-7	+1	
Q ₁	Q ₁	S ₂	-1	-1	-1		+1			-7
Q _{R12}	Q _{P21}	S ₁	(same NUBAR as Q ₁)		-1	+1		-7	0	
R ₂	P ₂	S ₁	+1	+1	+1	+1		-7	0	
R _{Q21}	P _{Q12}	S ₂	(same NUBAR as R ₂ or P ₂)		+1		+1			-7
P ₁	R ₁	S ₁	-1	-1	+1	+1		-7	+1	
P _{Q12}	R _{Q21}	S ₂	(same NUBAR as P ₁ or R ₁)		+1		-1			+1

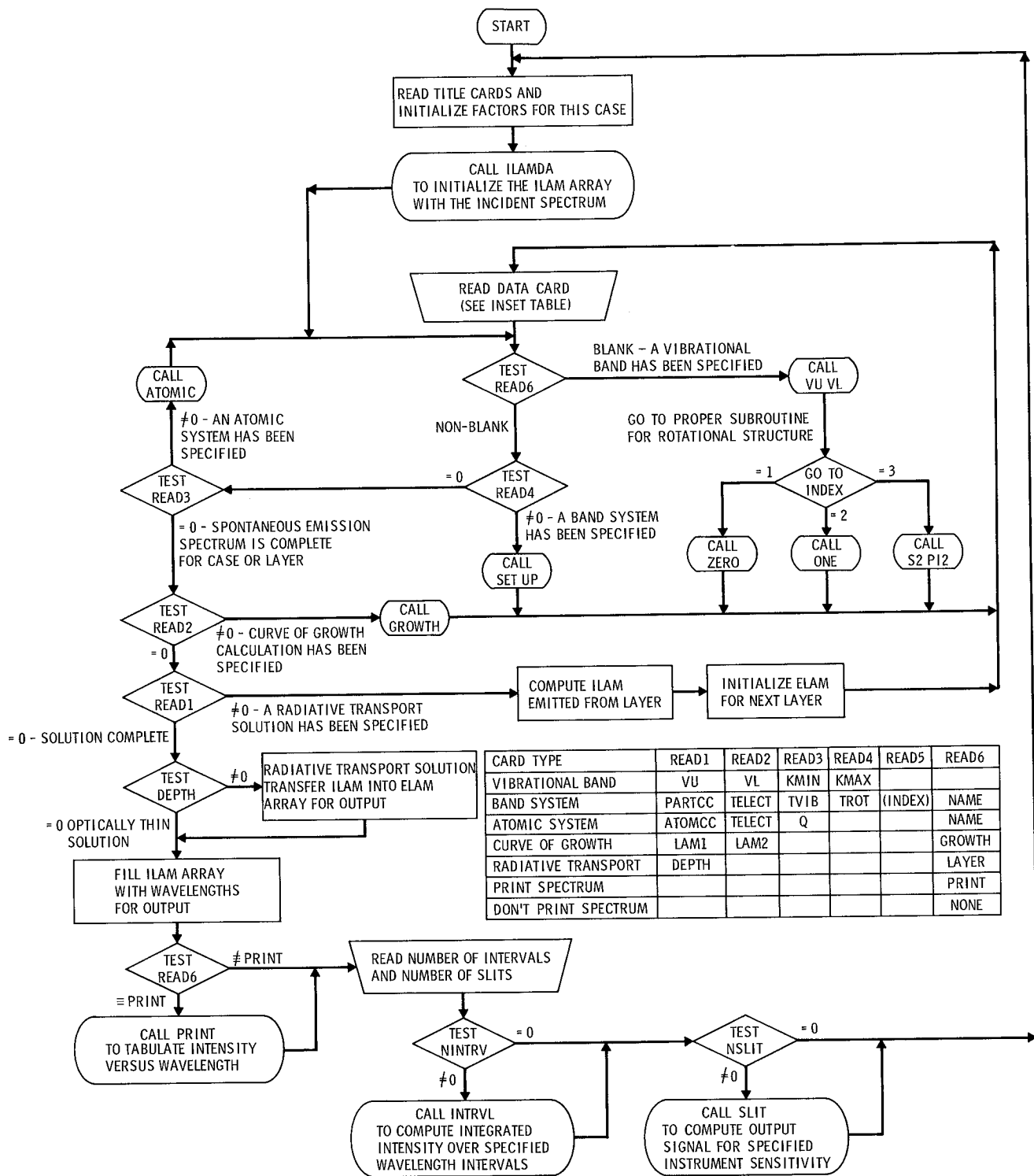


Figure 1.- Simplified flow chart of Main Program.

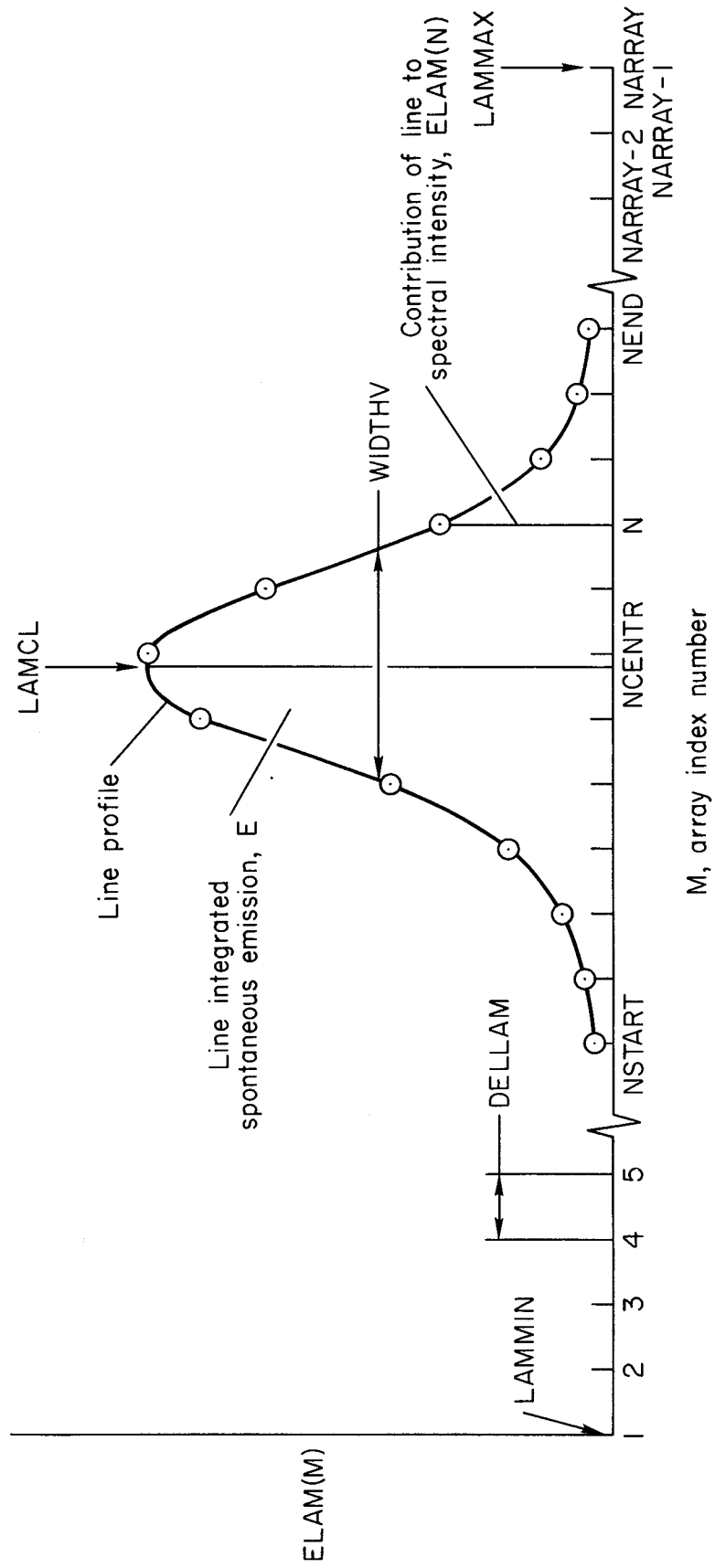


Figure 2.- Illustration of notation used in building the spontaneous-emission spectrum.

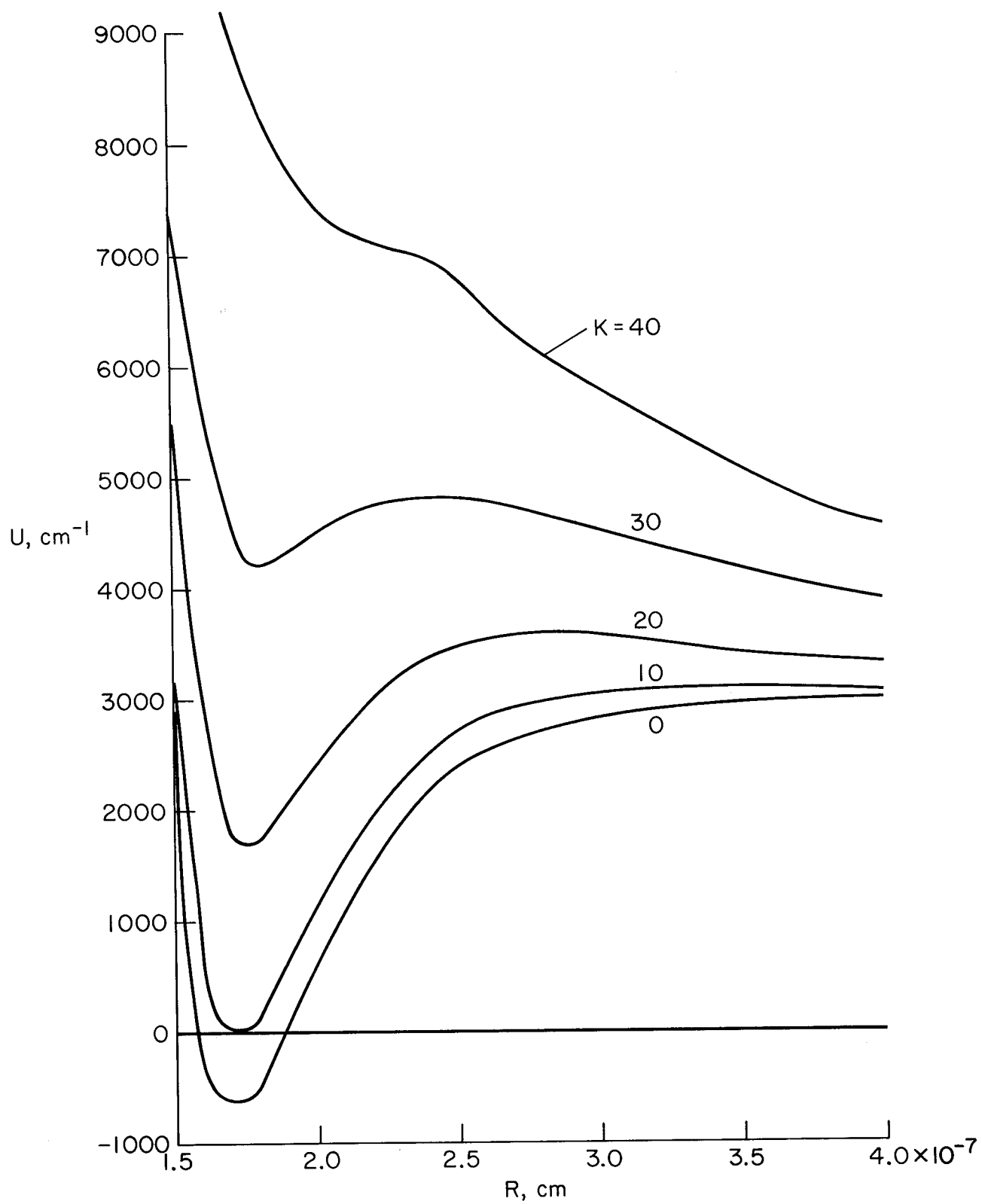


Figure 3.- Effective potential curves of HgH in the ground state. (Reproduced from ref. 9)

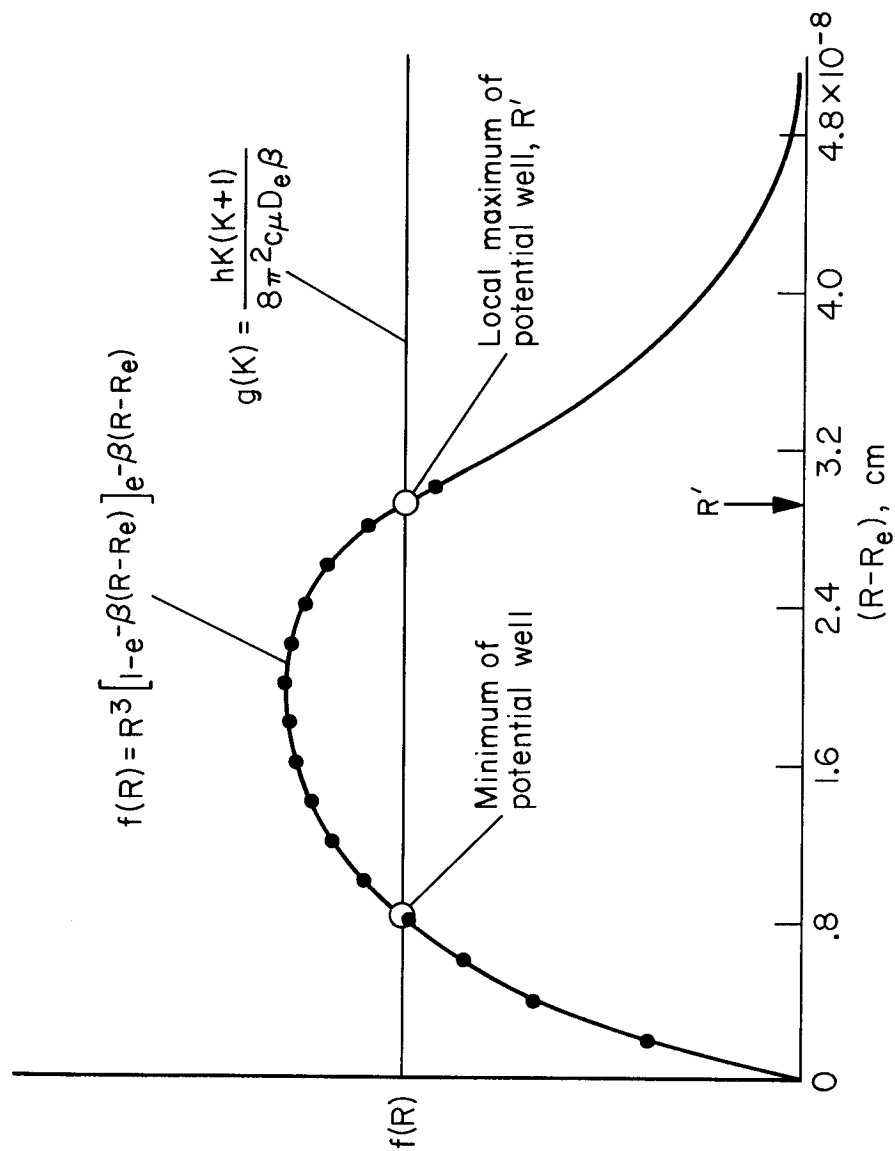


Figure 4.- Expressions used to find internuclear distance R' , at the local maximum of the potential well.

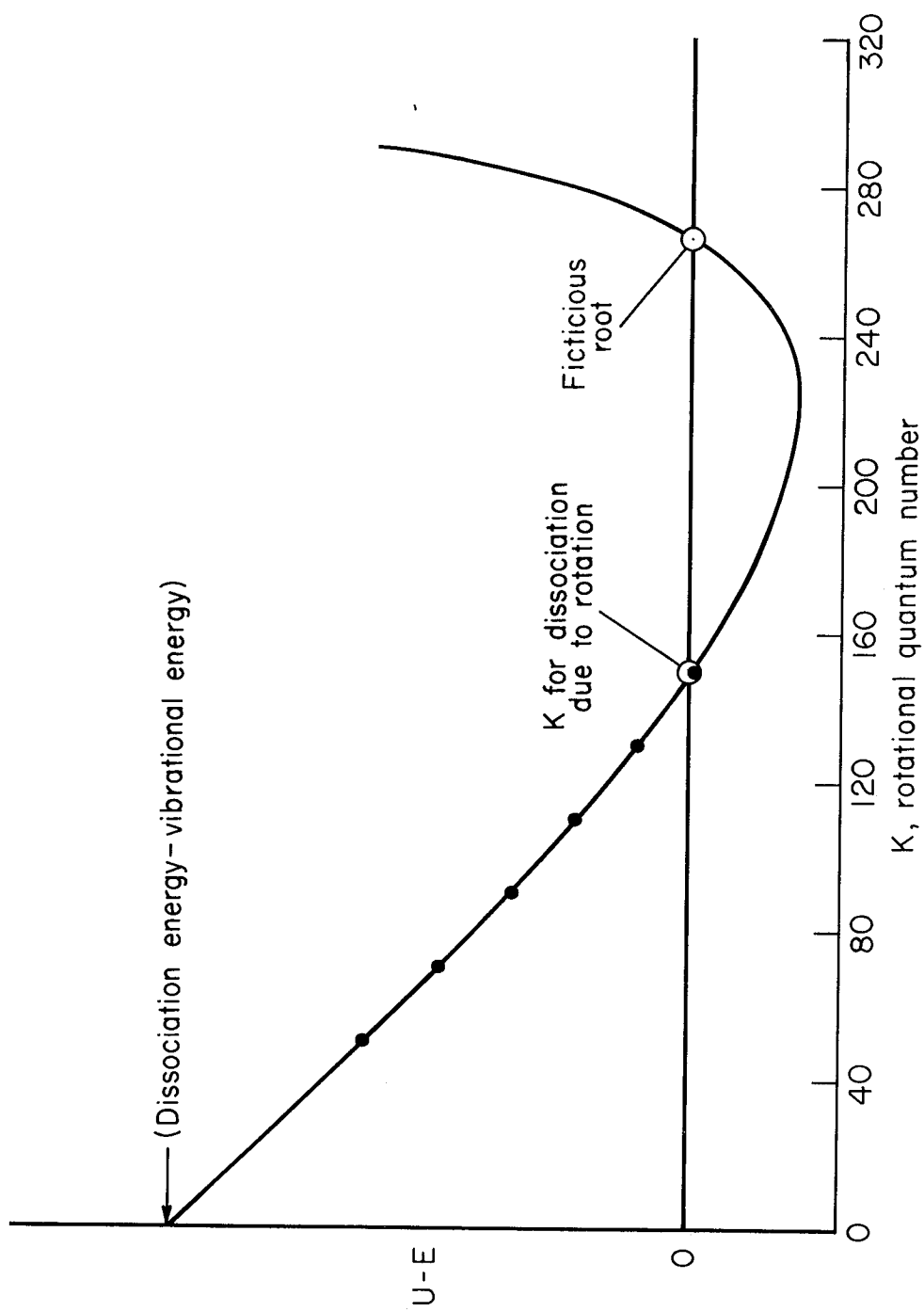


Figure 5.- Energy difference between local maximum of potential well and sum of vibrational and rotational energies.

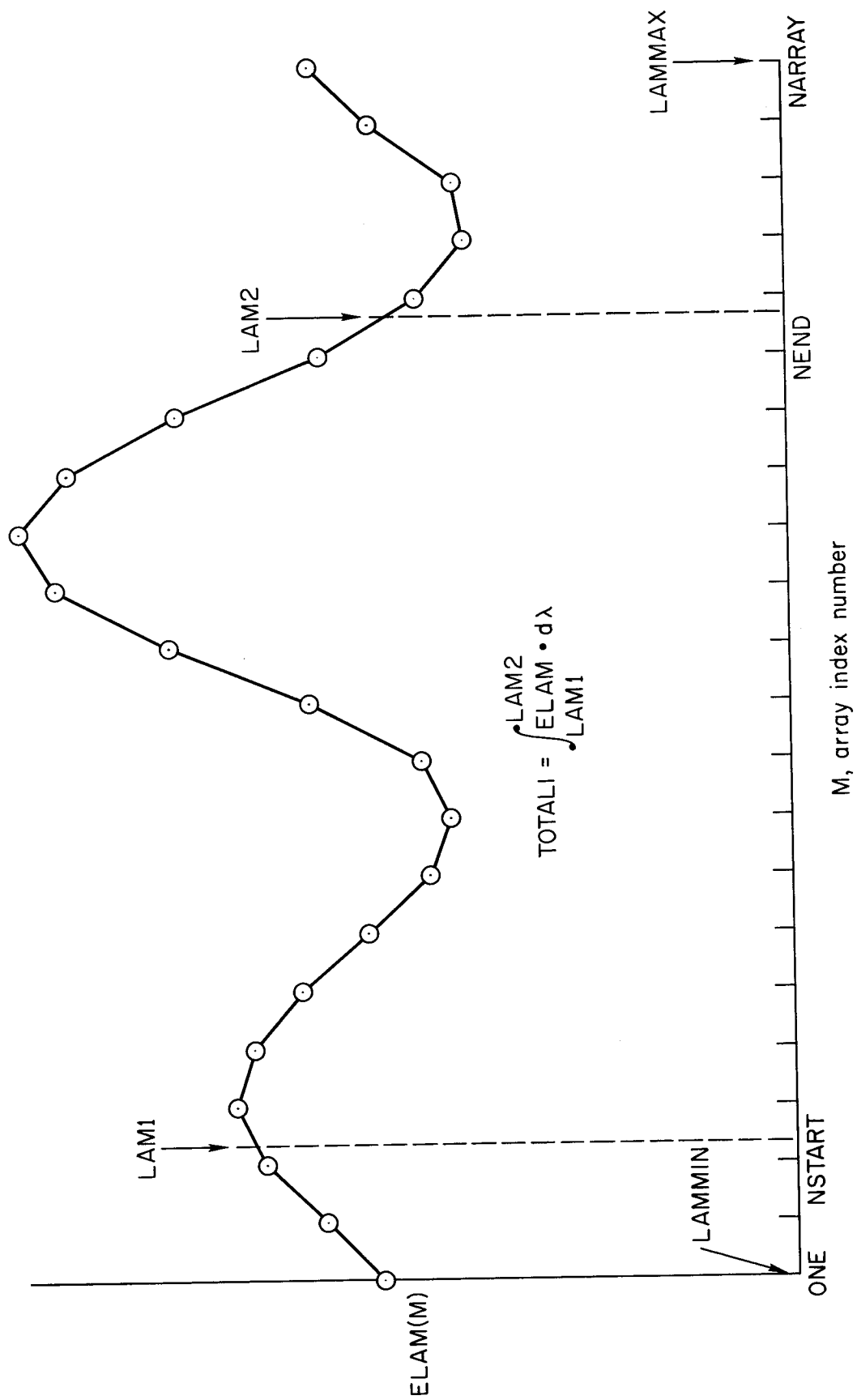
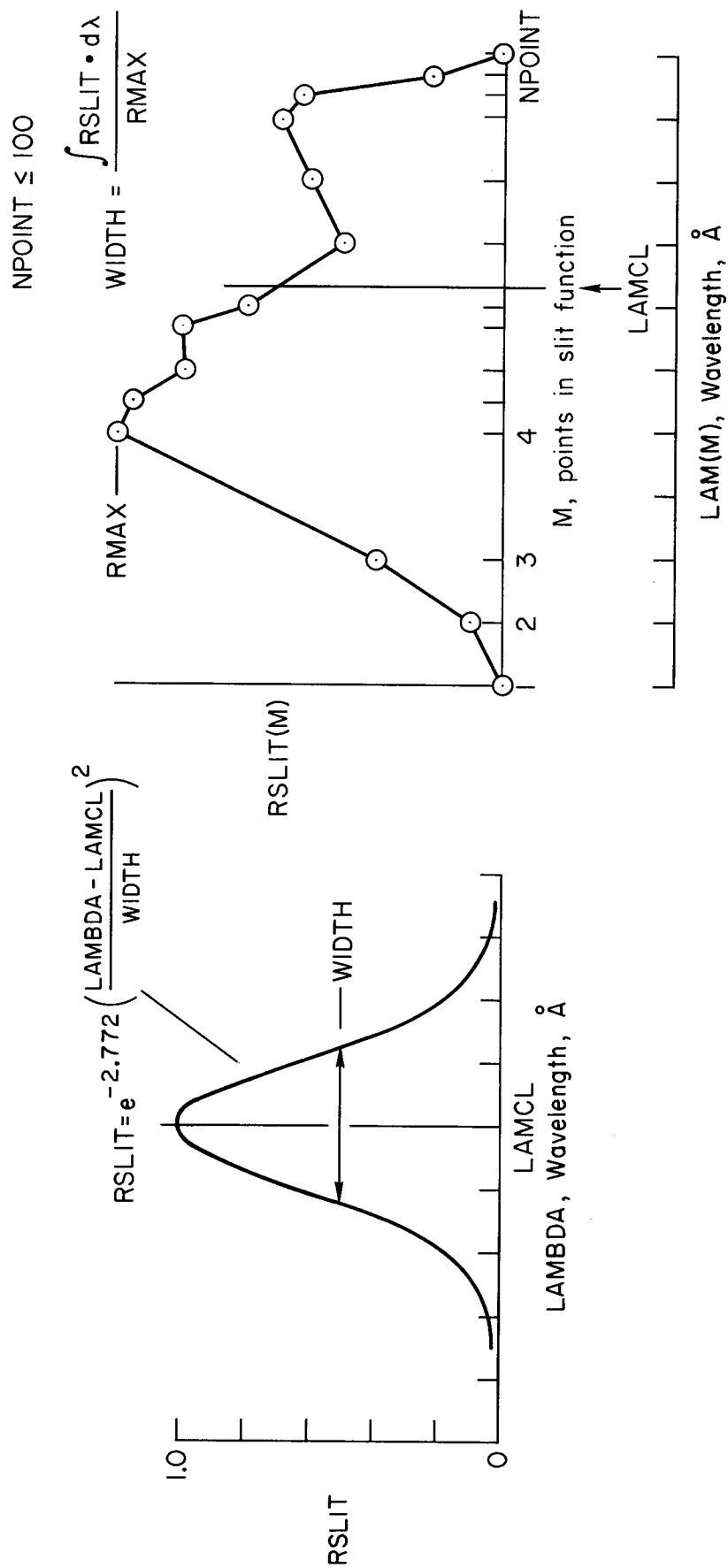


Figure 6.- Computed spectrum with integration limits.



(a) Gaussian slit function.

(b) Linear-segment slit function.

Figure 7.- Slit functions used in program.

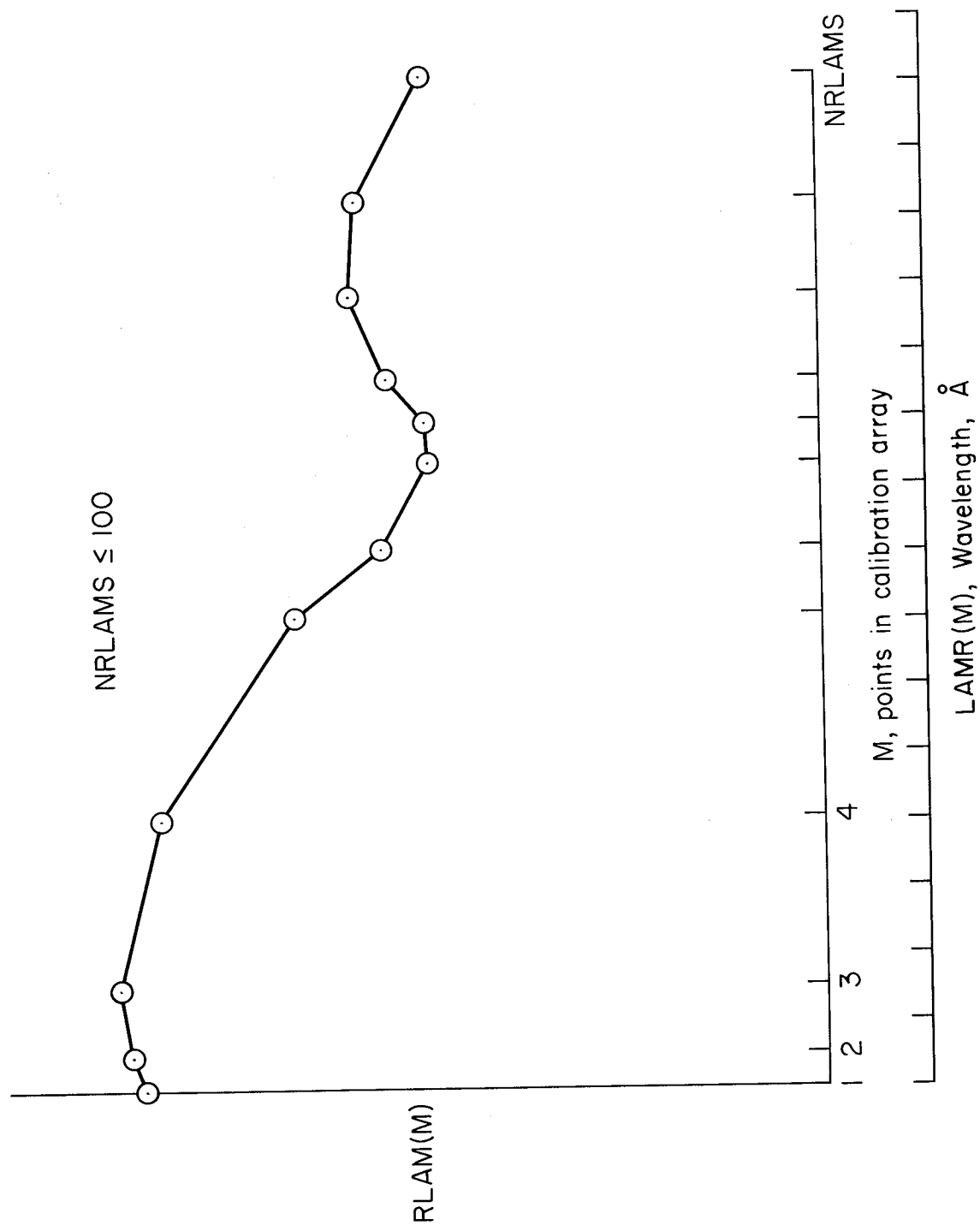


Figure 8.- Spectral calibration of grating spectrograph or scanning spectrometer.

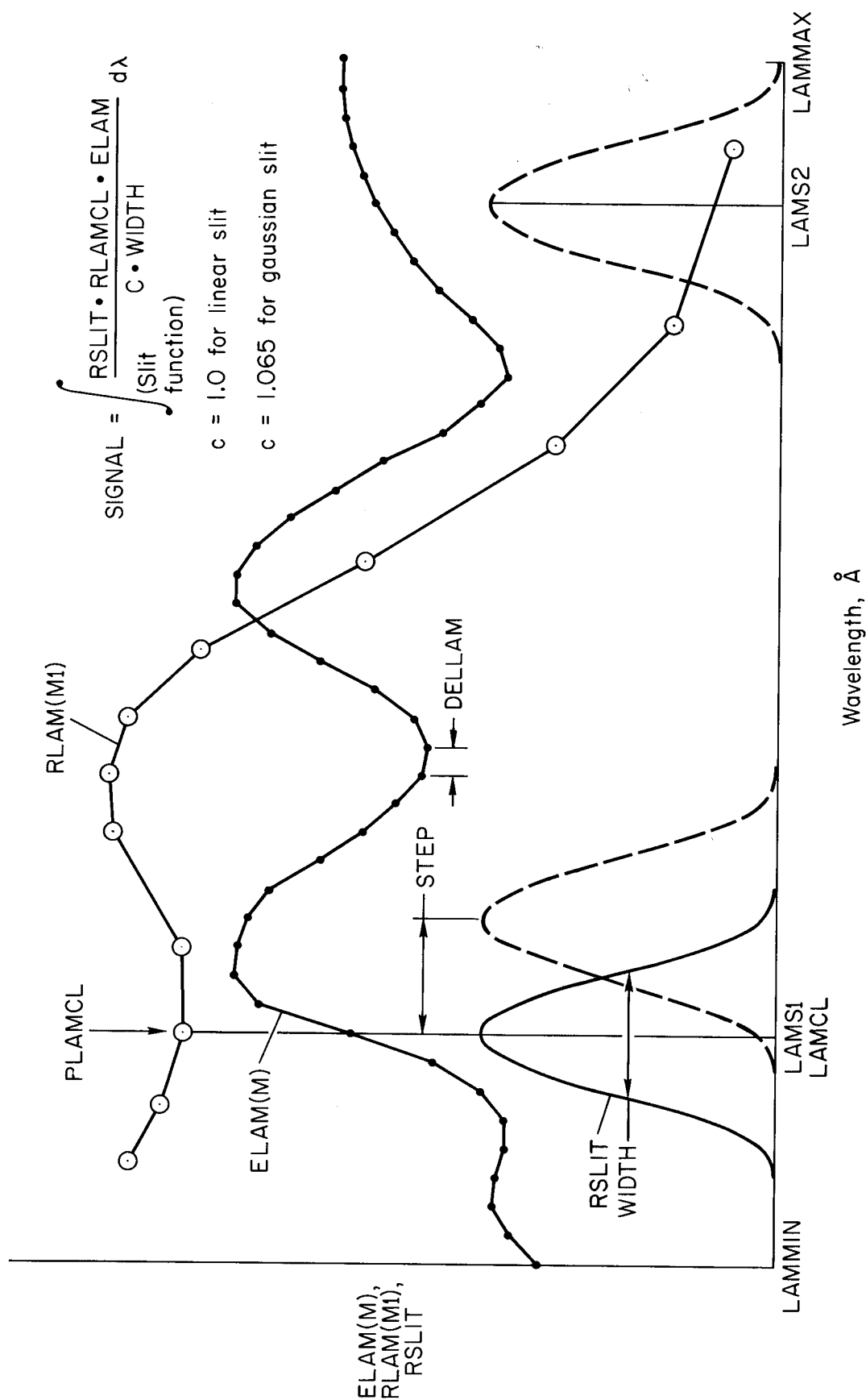


Figure 9.- Illustration of integration to produce instrument output signal.